FIGURE 3

LEGEND

Column headings from left to right are (A)'Atom Number', (B)'Atom Type', (C)'Amino Acid', (D)'Chain Identifier', (E)'Amino Acid Number', (F)'X Coordinate', (G)'Y Coordinate', (H)'Z Coordinate', (I)'Occupancy' (OCC) and (J)'B factor'.

A	В	С	D	Ε	F	G	Н	I	J
1	N	ALA	А	126	-1.22	5 18.275	58.949	1.00	62.30
2	CA	ALA			-0.16		59.906		61.70
3	CB	ALA			-0.35		60.315		62.19
4	C	ALA			-0.13		61.129		60.66
5	0	ALA			-0.94		62.044		61.53
6	N	ALA			0.78	4 16.805	61.123	1.00	59.08
7	CA	ALA			0.85	9 15.815	62.173	1.00	57.38
8	CB	ALA			1.25	5 14.482	61.599	1.00	57.77
9	С	ALA	Α	127	1.87	8 16.247	63.205	1.00	56.23
10	0	ALA	Α	127	3.07	5 16.075	63.000	1.00	56.65
11	N	TRP	Α	128	1.40	1 16.816	64.301	1.00	53.28
12	CA	TRP	Α	128	2.26	3 17.245	65.380	1.00	50.98
13	CB	TRP	Α	128	1.56	6 18.369	66.133	1.00	51.50
14	CG	TRP			1.40		65.268		52.38
15	CD1	TRP	Α	128	0.24	6 20.024	64.714	1.00	53.18
16	NE1	TRP			0.51		63.973		53.05
17	CE2	TRP			1.86		64.017		54.15
18	CD2	TRP	Α	128	2.44	2 20.405	64.834	1.00	53.19
19	CE3	TRP			3.82		65.049	1.00	
20	CZ3	TRP			4.55		64.458	1.00	
21	CH2	TRP			3.94		63.660		54.15
22	CZ2	TRP			2.60		63.431		54.51
23	С	TRP			2.51		66.332		49.09
24	0	TRP			1.74		66.370		48.80
25	N	ALA			3.59		67.100		47.28
26	CA	ALA			3.99		68.114		46.51
27	CB	ALA			5.02		67.555		45.67
28	C	ALA			4.59		69.262		45.56
29	0	ALA			4.98		69.037		43.83
30	N	LEU			4.65		70.480		46.03
31	CA	LEU			5.15		71.628		46.26
32	CB	LEU			5.11		72.909		46.46
33	CG	LEU			4.61		74.261		49.12
34	CD1	LEU			5.46		75.419		47.91
35	CD2	LEU			4.47		74.311		46.43
36 37	C	LEU			6.57 6.93		71.348		46.06 45.86
38							70.657		45.86
38	N CA	GLU			7.34 8.73		70.657		44.57
40	CB			131	9.50		69.669		45.34
41	CG			131	9.50		68.219	1.00	
41	CD	GLU		131	9.07		67.616	1.00	59.64

FIGURE 3A-(Cont.)

A	В	С	D	Ε	F	G	H	I	J
43	OE1	GLU	Α		8.836	13.078	66.726	1.00	64.32
44	OE2	GLU	Α	131	10.648	13.084	67.993	1.00	63.67
45	C	GLU	Α	131	8.937	17.577	69.485	1.00	41.74
46	0	GLU	Α	131	10.041	18.101	69.415	1.00	41.77
47	N	ASP	Α	132	7.881	18.078	68.841	1.00	39.05
48	CA	ASP	Α	132	8.010	19.323	68.100	1.00	38.32
49	CB	ASP	Α	132	6.935	19.466	67.028	1.00	39.96
50	CG	ASP	Α	132	6.946	18.299	66.066	1.00	41.30
51	OD1	ASP	Α	132	8.056	17.837	65.689	1.00	46.10
52	OD2	ASP	Α	132	5.894	17.772	65.723	1.00	42.94
53	C	ASP	Α	132	7.926	20.559	68.989	1.00	37.33
54	0	ASP	Α	132	8.094	21.640	68.472	1.00	36.39
55	N	PHE	Α	133	7.692	20.370	70.289	1.00	36.67
56	CA	PHE	Α	133	7.485	21.498	71.213	1.00	37.49
57	CB	PHE		133	5.998	21.569	71.740	1.00	36.30
58	CG	PHE	Α	133	4.958	21.474	70.656	1.00	38.62
59	CD1	PHE	Α	133	4.504	22.602	69.999	1.00	38.46
60	CE1	PHE	Α	133	3.564	22.499	68.993	1.00	41.24
61	CZ	PHE	Α	133	3.108	21.250	68.611	1.00	39.81
62	CE2	PHE			3.564	20.125	69.246	1.00	38.63
63	CD2	PHE			4.495	20.235	70.252	1.00	39.61
64	Ċ	PHE			8.475	21.593	72.399	1.00	38.04
65	Ó	PHE			8.934	20.578	72.922	1.00	37.77
66	N	GLU		134	8.825	22.817	72.801	1.00	37.74
67	CA	GLU		134	9.511	22.989	74.079	1.00	38.18
68	CB	GLU			10.583	24.031	73.989	1.00	38.70
69	CG	GLU			11.692	23.627	73.052	1.00	45.76
70	CD	GLU	Α	134	12.863	24.551	73.142	1.00	52.60
71	OE1	GLU			14.009	24.040	72.996	1.00	57.17
72	OE2	GLU	Α	134	12.635	25.768	73.380	1.00	57.77
73	C	GLU			8.424	23.456	74.979	1.00	37.78
74	Ó	GLU			7.697	24.400	74.647	1.00	37.67
75	N			135	8.295	22.825	76.123	1.00	35.90
76	CA	ILE		135	7.223	23.145	76.998	1.00	37.06
77	CB			135	6.657	21.878	77.499	1.00	37.79
78	CG1	ILE			5.960	21.157	76.334	1.00	41.64
79	CD1	ILE		135	4.794	20.341	76.792	1.00	48.55
80	CG2	ILE	Α	135	5.700	22.126	78.593	1.00	37.59
81	С	ILE	Α	135	7.682	24.058	78.152	1.00	36.78
82	0	ILE			8.778	23.906	78.672	1.00	34.54
83	N	GLY			6.819	24.998	78.533	1.00	37.69
84	CA	GLY			7.179	25.975	79.541	1.00	36.95
85	Ċ	GLY			6.383	25.807	80.792	1.00	37.86
86	Ó	GLY		136	6.052	24.706	81.139	1.00	38.85
87	N	ARG		137	6.052	26.917	81.449	1.00	38.75
88	CA	ARG		137	5.311	26.886	82.699	1.00	39.01
89	CB	ARG		137	5.392	28.252	83.369	1.00	40.79
90	CG	ARG		137	4.941	29.390	82.494	1.00	39.62
91	CD	ARG			4.835	30.762	83.163	1.00	45.72
92	NE	ARG		137	3.554	30.754	83.754		48.61

FIGURE 3

LEGEND

Column headings from left to right are (A)'Atom Number', (B)'Atom Type', (C)'Amino Acid', (D)'Chain Identifier', (E)'Amino Acid Number', (F)'X Coordinate', (G)'Y Coordinate', (H)'Z Coordinate', (I)'Occupancy' (OCC) and (J)'B factor'.

A	В	С	D	E		F		G		Н	I	J
1	N	ALA	Α	126	-:	1.225	1	18.275		58.949	1.00	62.30
2	CA			126		0.160		18.687		59.906		61.70
3	CB	ALA	Α	126	-0	3.351	- 2	20.162	4	60.315	1.00	62.19
4	С			126		0.137	1	17.763		51.129	1.00	
5	0	ALA	Α	126	- (940	1	17.908	4	62.044	1.00	61.53
6	N	ALA	Α	127		784	1	16.805	4	51.123	1.00	59.08
7	CA	ALA	Α	127		0.859	1	15.815	4	62.173	1.00	57.38
8	CB	ALA	Α	127		1.255	1	14.482	-	61.599	1.00	57.77
9	C	ALA	Α	127		1.878	1	16.247	-	63.205	1.00	56.23
10	0	ALA	Α	127		3.075	3	16.075		63.000	1.00	56.65
11	N	TRP				1.401		16.816		64.301	1.00	53.28
12	CA	TRP	Α	128	- :	2.263	1	17.245	- 4	65.380	1.00	50.98
13	CB			128		1.566		18.369		66.133	1.00	51.50
14	CG			128		1.402		19.546		65.268	1.00	52.38
15	CD1			128		0.246		20.024		64.714	1.00	53.18
16	NE1	TRP				0.515		21.153		63.973	1.00	53.05
17	CE2	TRP				1.862		21.394		64.017	1.00	54.15
18	CD2	TRP				2.442		20.405		54.834	1.00	53.19
19	CE3	TRP				3.820		20.440		65.049	1.00	54.16
20	CZ3			128		1.554		21.416		54.458	1.00	53.73
21	CH2	TRP				3.949		22.391		53.660	1.00	54.15
22	CZ2	TRP				2.606		22.395		53.431	1.00	54.51
23	C	TRP				2.517		16.093		66.332	1.00	
24	0	TRP				1.747		15.154		56.370		48.80
25	N	ALA				3.598		16.200		67.100	1.00	
26	CA	ALA				3.992		15.236		58.114	1.00	
27	CB	ALA				5.028		14.287		67.555		45.67
28	С	ALA				1.596		16.072		59.262	1.00	
29 30	O N	ALA		130		4.980 4.659		17.220 15.530		59.037 70.480	1.00	43.83
31				130		5.155		16.302		70.480 71.628	1.00	46.03
32	CA			130		5.119		15.469		72.909	1.00	
33	CG			130		4.612		16.028		74.261	1.00	49.12
34	CD1	LEU				5.469		15.546		75.419	1.00	47.91
35	CD2	LEU				4.470		17.523		74.311	1.00	
36	C	LEU				5.570		16.796		71.348		46.06
37	0	LEU				5.933		17.927		71.722	1.00	
38	N	GLU				7.349		15.967		70.657	1.00	
39	CA	GLU		131		3.736		16.309		70.328		43.80
40	CB			131		9.506		15.118		59.669	1.00	45.34
41	CG			131		9.077		14.915		58.219	1.00	50.12
42	CD		A	131		9.560		13.599		57.616	1.00	59.64

FIGURE 3A

A	В	С	D	Ε		F	G	Н		I	J
43	OE1	GLU	Α	131	8	.836	13.078	66.	726	1.00	64.32
44	OE2	GLU	Α	131	10	.648	13.084	67.	993	1.00	63.67
45	C	GLU	Α	131	8	.937	17.577	69.	485	1.00	41.74
46	0	GLU	Α	131		.041	18.101	69.	415	1.00	41.77
47	N	ASP	Α	132	7	.881	18.078	68.	841	1.00	39.05
48	CA	ASP	Α	132	8	.010	19.323	68.	100	1.00	38.32
49	CB	ASP	Α	132	6	.935	19.466	67.	028	1.00	39.96
50	CG	ASP				.946	18.299	66.		1.00	41.30
51	OD1	ASP				.056	17.837	65.		1.00	46.10
52	OD2	ASP				.894	17,772	65.		1.00	42.94
53	C	ASP				.926	20.559	68.		1.00	37.33
54	Ó	ASP				.094	21.640	68.		1.00	36.39
55	N	PHE				.692	20.370	70.		1.00	36.67
56	CA	PHE			7	.485	21.498	71.:		1.00	37.49
57	CB	PHE	Α	133	5	.998	21.569	71.	740	1.00	36.30
58	CG	PHE	Α	133	4	.958	21.474	70.	656	1.00	38.62
59	CD1	PHE	Α	133	4	.504	22.602	69.	999	1.00	38.46
60	CE1	PHE	А	133	3	.564	22.499	68.	993	1.00	41.24
61	CZ	PHE	Α	133	3	.108	21.250	68.	611	1.00	39.81
62	CE2	PHE				.564	20.125	69.		1.00	38.63
63	CD2	PHE				.495	20.235	70.		1.00	39.61
64	C	PHE				.475	21.593	72.		1.00	38.04
65	Ó	PHE				.934	20.578	72.		1.00	37.77
66	N	GLU		134		.825	22.817	72.		1.00	37.74
67	CA	GLU				.511	22.989	74.		1.00	38.18
68	CB	GLU				.583	24.031	73.		1.00	38.70
69	CG	GLU	Α	134		.692	23.627	73.	052	1.00	45.76
70	CD	GLU	Α	134	12	.863	24.551	73.	142	1.00	52.60
71	OE1	GLU	Α	134	14	.009	24.040	72.	996	1.00	57.17
72	OE2	GLU	Α	134	12	.635	25.768	73.	380	1.00	57.77
73	C	GLU	Α	134	8	.424	23.456	74.	979	1.00	37.78
74	0	GLU	Α	134	7	.697	24.400	74.	647	1.00	37.67
75	N	ILE	Α	135	8	.295	22.825	76.	123	1.00	35.90
76	CA	ILE	Α	135	7	.223	23.145	76.	998	1.00	37.06
77	CB	ILE	Α	135	6	.657	21.878	77.	499	1.00	37.79
78	CG1	ILE	Α	135	5	.960	21.157	76.	334	1.00	41.64
79	CD1	ILE	Α	135	4	.794	20.341	76.	792	1.00	48.55
80	CG2	ILE	Α	135	5	.700	22.126	78.	593	1.00	37.59
81	C	ILE	Α	135	7	.682	24.058	78.	152	1.00	36.78
82	0	ILE	Α	135	8	.778	23.906	78.	672	1.00	34.54
83	N	GLY	Α	136	6	.819	24.998	78.	533	1.00	37.69
84	CA	GLY	Α	136	7	.179	25.975	79.	541	1.00	36.95
85	C	GLY	Α	136	6	.383	25.807	80.	792	1.00	37.86
86	0	GLY	Α	136	6	.052	24.706	81.	139	1.00	38.85
87	N	ARG	Α	137		.052	26.917	81.		1.00	38.75
88	CA	ARG	Α	137	5	.311	26.886	82.	699	1.00	39.01
89	CB	ARG	Α	137	5	.392	28.252	83.	369	1.00	40.79
90	CG	ARG				.941	29.390	82.		1.00	39.62
91	CD	ARG				.835	30.762	83.		1.00	45.72
92	NE	ARG	Α	137	3	.554	30.754	83.	754	1.00	48.61

FIGURE 3B

A	В	С	D	E	F	G	H	1	J
93	CZ	ARG	А	137	2.501	31.519	83.484	1.00	42.31
94	NH1	ARG		137	2.481	32.576	82.674	1.00	39.40
95	NH2	ARG	Α	137	1.423	31.205	84.148	1.00	40.08
96	C	ARG	Α	137	3.841	26.591	82.437	1.00	38.31
97	0	ARG	Α	137	3.319	26.884	81.363	1.00	35.25
98	N	PRO	Α	138	3.186	26.035	83.432	1.00	38.59
99	CA	PRO	Α	138	1.741	25.812	83.367	1.00	37.99
100	CB	PRO		138	1.416	25.119	84.688	1.00	38.79
101	CG	PRO		138	2.691	24.697	85.283	1.00	38.62
102	CD	PRO		138	3.782	25.569	84.712	1.00	40.69
103	С	PRO		138	1.059	27.163	83.333	1.00	37.95
104	0	PRO		138	1.369	28.068	84.123	1.00	36.30
105	N	LEU			0.165	27.313	82.368	1.00	37.66
106 107	CA	LEU	A	139 139	-0.617 -1.012	28.512 28.701	82.249 80.804	1.00	35.85
108	CG	LEU		139	0.147	29.153	79.918	1.00	35.08
109	CD1	LEU		139	-0.222	29.133	78.419	1.00	33.54
110	CD2	LEU		139	0.576	30.644	80.230	1.00	35.10
111	C	LEU		139	-1.861	28.421	83.112	1.00	36.45
112	0	LEU		139	-2.410	29.451	83.532	1.00	35.77
113	N	GLY		140	-2.322	27.205	83.377	1.00	36.33
114	CA	GLY		140	-3.533	27.031	84.172	1.00	36.31
115	C	GLY	Α	140	-3.900	25.579	84.428	1.00	37.85
116	0	GLY	Α	140	-3.285	24.651	83.886	1.00	38.33
117	N	LYS	Α	141	-4.872	25.372	85.301	1.00	38.89
118	CA	LYS	Α	141	-5.255	24.016	85.681	1.00	40.43
119	CB	LYS	Α	141	-5.479	23.905	87.204	1.00	41.81
120	CG		А	141	-4.305	23.314	88.006	1.00	47.61
121	CD	LYS		141	-4.581	23.141	89.534	1.00	54.52
122	CE	LYS		141	-4.243	24.411	90.322	1.00	58.25
123	NZ			141	-3.204	25.271	89.614	1.00	61.08
124	С		Α	141	-6.575	23.809	84.999	1.00	39.72
125	0	LYS		141	-7.461	24.608	85.185	1.00	39.23
126	N	GLY		142	-6.677 -7.934	22.773	84.167 83.523	1.00	39.64
127 128	CA C	GLY		142 142	-8.491	22.410 21.213	84.310	1.00	40.24
129	0		A	142	-7.897	20.741	85.294	1.00	41.10
130	N		A	143	-9.640	20.722	83.907	1.00	41.52
131	CA		A	143	-10.245	19.612	84.630	1.00	42.27
132	CB		A	143	-11.686	19.435	84.202	1.00	43.00
133	CG			143	-12.432	18.544	85.170	1.00	48.58
134	CD		Α	143	-13.719	18.034	84.570	1.00	52.87
135	CE	LYS	Α	143	-14.622	17.577	85.684	1.00	56.82
136	NZ	LYS	Α	143	-14.896	16.117	85.592	1.00	61.41
137	С	LYS	Α	143	-9.471	18.292	84.453	1.00	41.56
138	0	LYS	Α	143	-9.248	17.572	85.412	1.00	40.75
139	N		Α	144	-9.014	18.045	83.228	1.00	40.56
140	CA	PHE		144	-8.344	16.807	82.827	1.00	40.12
141	CB	PHE		144	-9.010	16.315	81.546	1.00	40.15
142	CG	PHE			-10.461	16.037	81.725	1.00	42.78
143	CD1	PHE	Α	144	-10.877	14.867	82.383	1.00	45.37

FIGURE 3C

A	В	С	D	E	F	G	Н	I	J
144	CE1	PHE	Α	144	-12.211	14.607	82.568	1.00	42.37
145	CZ	PHE	Α	144	-13,160	15.517	82.120	1.00	44.22
146	CE2	PHE	Α	144	-12.757	16.679	81.499	1.00	43.36
147	CD2	PHE	Α	144	-11.420	16.948	81.315	1.00	39.89
148	C	PHE	Α	144	-6.842	16.866	82.611	1.00	38.97
149	0	PHE	Α	144	-6.253	15.909	82.150	1.00	36.84
150	N	GLY		145	-6.208	17.962	83.020	1.00	37.37
151	CA	GLY	Α	145	-4.783	18.120	82.806	1.00	38.17
152	С	GLY	Α	145	-4.486	19.606	82.814	1.00	37.75
153	0	GLY		145	-5.404	20.395	82.853	1.00	38.54
154	N			146	-3.230	19.999	82.753	1.00	38.01
155	CA	ASN		146	-2.930	21.412	82.804	1.00	37.94
156	CB	ASN		146	-1.619	21.626	83.563	1.00	38.27
157 158	CG OD1	ASN	A	146 146	-1.718 -2.704	21.186	85.022 85.695	1.00	43.37
159	ND2	ASN		146	-0.698	20.506	85.499	1.00	48.99
160	C	ASN		146	-2.821	21.982	81.391	1.00	36.46
161	0	ASN		146	-2.732	21.209	80.411	1.00	35.01
162	N	VAL		147	-2.830	23.317	81.293	1.00	34.34
163	CA	VAL		147	-2.512	23.965	80.024	1.00	32.03
164	CB	VAL		147	-3.518	25.083	79.686	1.00	32.73
165	CG1	VAL	Α	147	-3.098	25.767	78.335	1.00	31.49
166	CG2	VAL		147	-4.929	24.556	79.623	1.00	33.51
167	C	VAL	Α	147	-1.081	24.524	80.153	1.00	32.07
168	0	VAL	Α	147	-0.748	25.168	81.197	1.00	31.84
169	N	TYR	Α	148	-0.227	24.312	79.148	1.00	29.65
170	CA	TYR		148	1.167	24.744	79.257	1.00	30.70
171	CB	TYR		148	2.135	23.546	79.082	1.00	30.68
172	CG	TYR		148	1.969	22.547	80.199	1.00	34.98
173	CD1	TYR		148	1.006	21.542	80.117	1.00	36.63
174	CE1	TYR		148	0.800	20.623	81.187	1.00	43.31
175	CZ	TYR		148	1.568	20.721	82.344	1.00	43.61
176	OH	TYR		148	1.362	19.826	83.394	1.00	45.34
177	CE2	TYR		148	2.513 2.719	21.730	82.456 81.356	1.00	43.40
178 179	CD2 C	TYR		148 148	1.532	22.648 25.740	78.197	1.00	40.12
180	0	TYR		148	1.079	25.648	77.054	1.00	30.72
181	N		A	149	2.386	26.675	78.554	1.00	30.08
182	CA	LEU	A	149	3.001	27.513	77.534	1.00	30.86
183	CB	LEU		149	3.880	28.526	78.247	1.00	32.09
184	CG	LEU		149	4.108	29.924	77.676	1.00	36.09
185	CD1	LEU		149	5.567	30.516	77.808	1.00	34.85
186	CD2	LEU		149	3.332	30.344	76.361	1.00	32.07
187	C	LEU	Α	149	3.902	26.615	76.717	1.00	29.91
188	0	LEU	Α	149	4.557	25.743	77.269	1.00	31.11
189	N	ALA		150	4.008	26.837	75.417	1.00	29.95
190	CA	ALA		150	4.879	25.986	74.645	1.00	29.87
191	CB	ALA		150	4.091	24.697	74.127	1.00	29.08
192	C	ALA		150	5.435	26.770	73.456	1.00	30.54
193	0	ALA		150	4.860	27.774	72.966	1.00	29.82
194	N	ARG	Α	151	6.558	26.299	72.990	1.00	30.55

FIGURE 3D

A	В	С	D	E	F	G	Н	1	J
195	CA	ARG	Α	151	7.164	26.847	71.809	1.00	32.81
196	CB	ARG	Α	151	8.465	27.561	72.162	1.00	33.58
197	CG	ARG	Α	151	8.864	28.606	71.141	1.00	34.41
198	CD	ARG	Α	151	10.216	29.272	71.493	1.00	37.68
199	NE	ARG	Α	151	11.314	28.358	71.774	1.00	41.98
200	CZ	ARG	Α	151	12.579	28.754	71.840	1.00	45.91
201	NH1	ARG	Α	151	12.855	30.033	71.642	1.00	45.17
202	NH2	ARG	Α	151	13.554	27.891	72.109	1.00	48.67
203	C	ARG	Α	151	7.393	25.735	70.792	1.00	33.58
204	0	ARG	Α	151	7.806	24.623	71.151	1.00	36.75
205	N	GLU	Α	152	6.998	26.037	69.557	1.00	35.31
206	CA	GLU	Α	152	7.214	25.150	68.433	1.00	38.01
207	CB	GLU		152	6.339	25.554	67.232	1.00	38.19
208	CG	GLU	Α	152	6.245	24.450	66.177	1.00	44.01
209	CD	GLU	А	152	7.475	24.363	65.241	1.00	48.90
210	OE1	GLU	А	152	7.735	25.334	64.489	1.00	52.00
211	OE2	GLU		152	8.192	23.320	65.250	1.00	51.05
212	С	GLU		152	8.677	25.296	68.065	1.00	37.84
213	0	GLU	Α	152	9.161	26.382	67.791	1.00	38.28
214	N		Α	153	9.392	24.200	68.043	1.00	39.21
215	CA	LYS	Α	153	10.819	24.306	67.841	1.00	42.09
216	CB	LYS	Α	153	11.481	22.967	68.153	1.00	42.63
217	CG	LYS	Α	153	11.928	22.851	69.590	1.00	48.61
218	CD	LYS	Α	153	11.539	21.510	70.175	1.00	55.42
219	CE	LYS	Α	153	11.720	20.374	69.179	1.00	60.62
220	NZ	LYS	Α	153	13.095	19.664	69.260	1.00	68.26
221	C	LYS	A	153	11.287	24.885	66.509	1.00	42.57
222	0	LYS	Α	153	12.262	25.589	66.449	1.00	43.65
223 224	N	GLN	Α	154 154	10.603 11.158	24.623 25.126	65.421 64.163	1.00	43.01
225	CA CB	GLN		154	10.676	24.231	63.015	1.00	44.19
226	CG		A	154	11.442	22.952	63.015	1.00	53.28
227	CD	GLN		154	11.408	22.213	61.740	1.00	60.70
228	OE1	GLN	A	154	10.328	21.982	61.174	1.00	66.15
229	NE2	GLN		154	12.586	21.838	61.246	1.00	64.53
230	C	GLN		154	10.856	26.600	63.884	1.00	41.49
231	Ö		A	154	11.660	27.356	63.358	1.00	42.67
232	N	SER		155	9.675	27.022	64.254	1.00	38.39
233	CA	SER		155	9.313	28.371	63.946	1.00	35.68
234	CB	SER		155	7.840	28.364	63.594	1.00	34.74
235	OG	SER		155	7.196	27.875	64.746	1.00	34.70
236	C	SER		155	9.532	29.313	65.140	1.00	33.68
237	0	SER		155	9.505	30.517	64.946	1.00	33.85
238	N	LYS	Α	156	9.672	28.739	66.331	1.00	32.82
239	CA	LYS	Α	156	9.704	29.445	67.645	1.00	34.59
240	CB	LYS	Α	156	10.858	30.467	67.753	1.00	34.66
241	CG	LYS	Α	156	12.319	29.876	67.480	1.00	36.79
242	CD	LYS	Α	156	13.429	30.907	67.970	1.00	44.57
243	CE	LYS	Α	156	14.696	31.115	67.056	1.00	47.52
244	NZ	LYS		156	14.787	32.563	66.539	1.00	46.31
245	C	LYS	Α	156	8.335	30.102	67.987	1.00	33.10

FIGURE 3E

A	В	C	D	E	F	G	H	1	J
246	0	LYS	Α	156	8.218	31.065	68.804	1.00	31.56
247	N	PHE	Α	157	7.302	29.553	67.386	1.00	31.13
248	CA	PHE	Α	157	5.948	30.020	67.646	1.00	31.45
249	CB	PHE	Α	157	5.016	29.469	66.575	1.00	32.15
250	CG	PHE	Α	157	3.713	30.177	66.469	1.00	34.87
251	CD1	PHE	Α	157	3.527	31.155	65.492	1.00	38.48
252	CE1	PHE	Α	157	2.274	31.786	65.329	1.00	40.08
253	CZ	PHE	Α	157	1.209	31.427	66.143	1.00	37.15
254	CE2	PHE	Α	157	1.368	30.425	67.104	1.00	34.69
255	CD2	PHE	Α	157	2.644	29.795	67.253	1.00	36.13
256	C	PHE	Α	157	5.466	29.641	69.057	1.00	29.29
257	0	PHE	Α	157	5.395	28.469	69.412	1.00	29.48
258	N	ILE		158	5.022	30.656	69.813	1.00	29.61
259	CA	ILE	Α	158	4.651	30.447	71.207	1.00	30.50
260	CB	ILE	Α	158	4.899	31.717	72.032	1.00	31.00
261	CG1		А	158	6.366	31.797	72.339	1.00	36.27
262	CD1	ILE		158	6.687	30.925	73.512	1.00	37.94
263	CG2	ILE	Α	158	4.419	31.510	73.466	1.00	32.23
264	C	ILE		158	3.209	30.163	71.230	1.00	29.07
265	0			158	2.473	30.911	70.644	1.00	30.88
266	N	LEU		159	2.745	29.157	71.935	1.00	28.37
267	CA	LEU			1.339	28.868	71.885	1.00	28.41
268	CB	LEU		159	1.085	27.936	70.692	1.00	28.97
269	CG	LEU		159	1.953	26.777	70.259	1.00	34.00
270	CD1	LEU		159	1.782	25.602	71.203	1.00	35.94
271	CD2	LEU		159	1.737	26.341	68.787	1.00	39.02
272	С	LEU		159	1.079	28.193	73.204	1.00	27.83
273	0	LEU		159	1.957	28.166	74.034	1.00	27.51
274	N	ALA		160	-0.120	27.685	73.409	1.00	29.15
275 276	CA	ALA		160 160	-0.450 -1.651	27.016 27.684	74.661 75.323	1.00	30.37
277		ALA			-0.818		74.297	1.00	28.84
278	C	ALA		160	-1.472	25.602 25.371	73.269	1.00	32.10
279	N	LEU		161	-0.434	24.654	75.163	1.00	33.02
280	CA	LEU		161	-0.741	23.261	74.941	1.00	34.14
281	CB	LEU		161	0.577	22.495	74.913	1.00	34.88
282	CG	LEU		161	0.908	21.455	73.868	1.00	39.45
283	CD1		A	161	0.455	21.854	72.442	1.00	35.63
284	CD2	LEU		161	2.466	21.138	73.933	1.00	40.14
285	C	LEU		161	-1.648	22.780	76.036	1.00	33.03
286	ō	LEU		161	-1.271	22.762	77.217	1.00	33.04
287	N	LYS		162	-2.885	22.456	75.657	1.00	31.43
288	CA		Α	162	-3.856	21.979	76.610	1.00	32.34
289	CB		Α	162	-5.251	22.451	76.196	1.00	32.99
290	CG	LYS	Α	162	-6.391	21.951	77.087	1.00	29.62
291	CD		Α	162	-7.595	22.831	76.855	1.00	29.33
292	CE	LYS		162	-8.841	22.204	77.533	1.00	27.32
293	NZ	LYS		162	-10.098	22.987	77.412	1.00	31.96
294	C	LYS	Α	162	-3.772	20.441	76.654	1.00	33.11
295	0	LYS		162	-4.017	19.775	75.666	1.00	33.31
296	N	VAL	Α	163	-3.364	19.907	77.790	1.00	35.02

FIGURE 3F

A	В	С	D	E	F	G	H	I	J
297	CA	VAL	Α	163	-3.205	18.471	77.983	1.00	37.14
298	CB	VAL	Α	163	-1.971	18.203	78.854	1.00	36.58
299	CG1	VAL	Α	163	-1.720	16.660	79.039	1.00	37.74
300	CG2	VAL	Α	163	-0.709	18.909	78.260	1.00	38.41
301	C	VAL	Α	163	-4.445	17.854	78.653	1.00	37.59
302	0	VAL	Α	163	-4.960	18.395	79.644	1.00	37.22
303	N	LEU		164	-4.977	16.767	78.073	1.00	39.14
304	CA	LEU		164	-6.104	16.048	78.686	1.00	39.01
305	CB	LEU		164	-7.427	16.202	77.930	1.00	39.22
306	CG	LEU		164	-7.961	17.622	77.781	1.00	38.09
307	CD1		Α	164	-7.363	18.125	76.508	1.00	38.01
308	CD2	LEU		164	-9.453	17.647	77.711	1.00	37.35
309	С	LEU		164	-5.759	14.562	78.783	1.00	39.97
310	0	LEU		164	-5.369	13.952	77.798	1.00	38.76
311	N		Α	165	-5.880 -5.535	14.004	79.986	1.00	40.67
312 313	CA		A	165	-5.535 -5.191	12.599	80.211	1.00	42.42
313	CB	PHE	A A	165 165	-3.815	12.355 12.784	81.686 82.030	1.00	42.83
315	CD1	PHE		165	-3.573	14.040	82.560	1.00	47.62
316	CE1	PHE		165	-2.290	14.434	82.868	1.00	47.96
317	CZ	PHE		165	-1.227	13.574	82.628	1.00	50.56
318	CE2	PHE		165	-1.446	12.349	82.067	1.00	48.72
319	CD2			165	-2.740	11.951	81.775	1.00	48.08
320	C	PHE		165	-6.665	11.709	79.743	1.00	42.46
321	Ö	PHE		165	-7.788	11.832	80.199	1.00	40.57
322	N		А	166	-6.360	10.867	78.768	1.00	43.35
323	CA		А	166	-7.342	9.957	78.209	1.00	45.50
324	CB	LYS	Α	166	-6.696	9.043	77.155	1.00	46.27
325	CG	LYS	Α	166	-6.559	9.666	75.786	1.00	46.27
326	CD	LYS	Α	166	-5.423	8.956	75.032	1.00	53.89
327	CE	LYS	Α	166	-5.279	9.445	73.581	1.00	55.13
328	NZ	LYS		166	-5.709	8.444	72.569	1.00	59.86
329	C		Α	166	-8.040	9.102	79.273	1.00	45.98
330	0	LYS		166	-9.230	8.981	79.250	1.00	46.56
331	N	ALA		167	-7.324	8.561	80.240	1.00	47.94
332	CA	ALA		167	-8.025	7.699	81.191	1.00	49.17
333	CB	ALA		167	-7.091	7.201	82.220	1.00	49.16
334	С	ALA		167	-9.168	8.457	81.848	1.00	49.92
335	0	ALA		167	-10.305	7.957	81.995	1.00	49.78
336	N	GLN		168	-8.859	9.696	82.218	1.00	49.84
337	CA	GLN		168	-9.787	10.502	82.960	1.00	49.29
338 339	CB	GLN		168	-9.058	11.694	83.591	1.00	50.22
340	CG	GLN		168 168	-8.451 -7.028	11.419 10.830	84.993 84.965	1.00	54.78 62.45
341	OE1		A	168	-6.053	11.569	84.788	1.00	65.02
342	NE2	GLN		168	-6.908	9.511	85.190	1.00	64.80
343	C	GLN		168	-10.953	10.939	82.088	1.00	48.29
344	0	GLN		168	-12.085	10.976	82.553	1.00	47.87
345	N	LEU		169	-10.702	11.245	80.814	1.00	48.22
346	CA		A	169	-11.808	11.676	79.964	1.00	48.39
347	CB	LEU		169	-11.322	12.112	78.575	1.00	47.89

FIGURE 3G

A	В	С	D	E	F	G	Н	1	J
348	CG	LEU	Α	169	-10.644	13.461	78.330	1.00	49.67
349	CD1	LEU	Α	169	-10.181	13.552	76.882	1.00	48.91
350	CD2	LEU	Α	169	-11.615	14.580	78.615	1.00	45.84
351	C	LEU	Α	169	-12.819	10.538	79.785	1.00	47.86
352	0	LEU		169	-14.027	10.733	79.875	1.00	47.83
353	N	ALA		170	-12.316	9.368	79.451	1.00	48.31
354	CA	ALA		170	-13.220	8.238	79.195	1.00	48.55
355	CB	ALA		170	-12.468	7.070	78.581	1.00	49.34
356	С	ALA		170	-13.927	7.860	80.494	1.00	48.26
357	0	ALA		170	-15.118	7.692	80.501	1.00	49.17
358	N	ALA		171 171	-13.207	7.806 7.578	81.606	1.00	48.63
359 360	CA	ALA		171	-13.857 -12.858	7.685	82.885 84.058	1.00	48.78
361	C	ALA		171	-14.996	8.561	83.082	1.00	48.71
362	0	ALA		171	-16.113	8.179	83.429	1.00	48.35
363	N	ALA		172	-14.723	9.841	82.844	1.00	48.29
364	CA	ALA		172	-15.740	10.846	83.012	1.00	47.44
365	CB	ALA		172	-15.093	12.246	83.064	1.00	48.07
366	C	ALA		172	-16.759	10.737	81.888	1.00	47.98
367	ō	ALA		172	-17.893	11.232	81.984	1.00	48.40
368	N	GLY	Α	173	-16.371	10.067	80.815	1.00	48.12
369	CA	GLY	Α	173	-17.262	9.907	79.674	1.00	47.85
370	C	GLY	Α	173	-17.733	11.166	78.995	1.00	47.73
371	0	GLY	Α	173	-18.926	11.308	78.705	1.00	49.07
372	N	VAL	Α	174	-16.790	12.075	78.736	1.00	46.88
373	CA	VAL		174	-17.030	13.322	78.021	1.00	45.99
374	CB	VAL		174	-16.674	14.572	78.873	1.00	45.74
375	CG1	VAL		174	-17.722	14.810	79.913	1.00	49.76
376	CG2	VAL		174	-15.330	14.425	79.472	1.00	46.00
377	С	VAL		174	-16.132	13.394	76.798	1.00	44.25
378	0	VAL		174	-15.792	14.483	76.300	1.00	43.32
379	N	ALA		175	-15.708 -14.879	12.236 12.221	76.322 75.125	1.00	42.33
380 381	CA	ALA		175 175	-14.563	10.748	74.679	1.00	41.82
382	C	ALA		175	-15.577	13.026	74.008	1.00	40.98
383	Ö	ALA		175	-14.920	13.683	73.189	1.00	42.44
384	N	HIS	A	176	-16.899	13.030	74.009	1.00	40.16
385	CA	HIS	A	176	-17.657	13.751	72.980	1.00	41.39
386	CB	HIS	A	176	-19.146	13.385	73.068	1.00	41.58
387	CG		A	176	-19.803	13.903	74.318	1.00	45.86
388	ND1	HIS	Α	176	-19.695	13.259	75.543	1.00	47.14
389	CE1	HIS	Α	176	-20.355	13.949	76.460	1.00	47.79
390	NE2	HIS	Α	176	-20.854	15.035	75.885	1.00	49.44
391	CD2	${\tt HIS}$	Α	176	-20.532	15.023	74.545	1.00	46.34
392	C	HIS	Α	176	-17.477	15.312	73.096	1.00	40.21
393	0	HIS	Α	176	-17.529	16.043	72.107	1.00	38.56
394	N	GLN	Α	177	-17.282	15.793	74.320	1.00	39.05
395	CA	GLN	Α	177	-17.021	17.231	74.544	1.00	39.77
396	CB	GLN	Α	177	-17.008	17.567	76.019	1.00	38.88
397	CG	GLN		177	-18.343		76.675	1.00	38.17
398	CD	GLN	Α	177	-18.467	17.978	78.032	1.00	36.45

FIGURE 3H

Α	В	С	D	Ε	F	G	Н	I	J
399	OE1	GLN	Α	177	-19.5	.436	78.382	1.00	43.55
400	NE2	GLN		177	-17.3	992	78.801	1.00	32.42
401	C	GLN		177	-15.6	.586	73.966	1.00	39.55
402	0	GLN	Α	177	-15.5	636	73.379	1.00	40.58
403	N	LEU		178	-14.6	.722	74.144	1.00	38.53
404	CA		Α	178	-13.3	.016	73.556	1.00	38.40
405	CB	LEU	Α	178	-12.3	.028	73.974	1.00	37.56
406	CG	LEU	Α	178	-10.9	463	73.548	1.00	39.19
407	CD1	LEU		178	-10.6	912	74.074	1.00	42.88
408	CD2	LEU	Α	178	-9.8	.543	74.112	1.00	42.48
409	C	LEU		178	-13.5	.041	72.039	1.00	38.85
410	0	LEU		178	-12.9	902	71.384	1.00	38.48
411	N	ARG		179	-14.3	.156	71.478	1.00	38.80
412	CA	ARG		179	-14.5	.156	70.027	1.00	38.95
413	CB	ARG		179	-15.5	.134	69.583	1.00	41.23
414	CG	ARG		179	-15.2	622	68.199	1.00	45.48
415	CD	ARG		179	-15.3	.090	68.099	1.00	56.58
416	NE	ARG		179	-16.4	637	69.012	1.00	57.68
417	CZ	ARG		179	-16.2	730	69.973	1.00	57.26
418	NH1	ARG		179	-17.2	.381	70.749	1.00	53.81
419	NH2	ARG		179	-15.0	.162	70.159	1.00	59.58
420	C	ARG			-15.0	456	69.558	1.00	38.62
421	0	ARG		179	-14.7	995	68.508	1.00	38.21
422	N	ARG		180	-16.0	943	70.318	1.00	39.35
423	CA	ARG		180	-16.7	.126	69.851	1.00	41.02
424	CB	ARG		180	-18.0	.338	70.575	1.00	41.10
425	CG	ARG		180	-19.3	248	69.686	1.00	48.65
426	CD	ARG		180	-20.3	.182	70.125	1.00	56.75
427	NE	ARG		180	-20.6	254	71.551	1.00	60.82
428	CZ	ARG		180	-21.7	.672	72.127	1.00	64.30
429	NH1	ARG		180	-21.9	.819	73.430	1.00	64.17
430	NH2	ARG			-22.5	958	71.400	1.00	65.87
431	С	ARG		180	-15.8	374	69.923	1.00	39.65
432	0	ARG		180	-15.9	204	69.026	1.00	38.25
433 434	N	GLU		181	-15.1 -14.3	.501	71.003	1.00	39.01
434	CA CB	GLU		181 181	-14.3	.665 .368	72.514	1.00	38.98
436	CG	GLU	A	181	-12.4	.429	72.937	1.00	41.25
437	CD	GLU		181	-11.9	.254	74.396	1.00	44.88
437	OE1	GLU		181	-10.9	921	74.792	1.00	48.21
439	OE2	GLU		181	-10.5	477	75.192	1.00	45.90
440	C	GLU		181	-13.3	802	70.074	1.00	38.90
441	Ö	GLU		181	-13.1	.894	69.576	1.00	38.31
442	N	VAL		182	-12.8	.667	69.651	1.00	38.34
443	CA	VAL		182	-11.8	639	68.537	1.00	38.73
444	CB	VAL		182	-11.0	.274	68.390	1.00	40.09
445	CG1	VAL		182	-10.4	.128	66.980	1.00	40.39
446	CG2	VAL		182	-10.0	.079	69.506	1.00	38.26
447	C	VAL		182	-12.5	959	67.237	1.00	38.65
448	Ö	VAL		182	-12.1	.839	66.516	1.00	39.07
449	N	ALA		183	-13.6	285	66.957	1.00	39.36

FIGURE 3I

A	В	C	D	E		F	G	H	1	J
450	CA	ALA	Α	183	-14.		20.503	65.679	1.00	40.14
451	CB	ALA		183	-15.		19.370	65.405	1.00	41.08
452	C	ALA	Α	183	-14.		21.870	65.636	1.00	40.80
453	0	ALA	Α	183	-14.		22.545	64.609	1.00	41.84
454	N	ILE	Α	184	-15.	524	22.312	66.748	1.00	38.99
455	CA	ILE	Α	184	-16.	157	23.595	66.678	1.00	39.48
456	CB	ILE	Α	184	-17.	210	23.754	67.766	1.00	38.90
457	CG1	ILE	Α	184	-18.	387	22.819	67.472	1.00	42.19
458	CD1	ILE	Α	184	-19.	459	22.799	68.584	1.00	40.68
459	CG2	ILE	Α	184	-17.	715	25.164	67.777	1.00	40.73
460	C	ILE	Α	184	-15.	124	24.703	66.747	1.00	39.32
461	0	ILE	Α	184	-15.	148	25.635	65.929	1.00	38.88
462	N	GLN	Α	185	-14.	209	24.612	67.723	1.00	38.82
463	CA	GLN	Α	185	-13.	281	25.717	67.911	1.00	38.20
464	CB	GLN	Α	185	-12.	446	25.531	69.185	1.00	38.61
465	CG	GLN	Α	185	-12.	426	26.806	70.015	1.00	36.79
466	CD	GLN	Α	185	-11.	623	26.663	71.277	1.00	38.97
467	OE1	GLN	Α	185	-10.	817	27.519	71.599	1.00	35.32
468	NE2	GLN	Α	185	-11.	869	25.627	71.997	1.00	32.38
469	C	GLN	Α	185	-12.	337	25.905	66.754	1.00	38.81
470	0	GLN	Α	185	-11.	936	27.027	66.479	1.00	37.38
471	N	SER	Α	186	-11.	946	24.823	66.083	1.00	39.57
472	CA	SER	Α	186	-10.	957	25.005	65.007	1.00	41.86
473	CB	SER	Α	186	-10.	302	23.684	64.569	1.00	41.93
474	OG	SER	Α	186	-11.	289	22.671	64.412	1.00	42.48
475	С	SER	Α	186	-11.	509	25.748	63.798	1.00	42.50
476	0	SER	Α	186	-10.	761	26.297	63.017	1.00	43.08
477	N	HIS	Α	187	-12.	817	25.781	63.656	1.00	43.53
478	CA	HIS	Α	187	-13.		26.411	62.471	1.00	45.61
479	CB		Α	187	-14.	585	25.580	61.955	1.00	46.41
480	CG	HIS	Α	187	-14.		24.264	61.396	1.00	52.65
481	ND1	HIS	Α	187	-14.	352	23.934	60.072	1.00	58.39
482	CE1	HIS	Α	187	-13.		22.725	59.855	1.00	58.68
483	NE2	HIS	Α	187	-13.	354	22.269	60.986	1.00	59.03
484	CD2	HIS	Α	187	-13.		23.215	61.965	1.00	56.31
485	C	HIS	А	187	-13.		27.843	62.684	1.00	44.76
486	ō		А	187	-13.		28.608	61.725	1.00	44.78
487	N	LEU	А	188	-13.		28.229	63.945	1.00	44.38
488	CA	LEU	A	188	-14.		29.612	64.257	1.00	43.43
489	CB	LEU		188	-14.		29.748	65.747	1.00	43.01
490	CG	LEU	Α	188	-15.		28.891	66.146	1.00	43.56
491	CD1	LEU		188	-16.		29.051	67.640	1.00	41.71
492	CD2	LEU		188	-17.		29.282	65.302	1.00	41.54
493	C	LEU	A	188	-13.		30.477	64.001	1.00	42.37
494	Ö	LEU		188	-12.		30.079	64.321	1.00	43.11
495	N		A	189	-13.		31.677	63.478	1.00	42.12
496	CA	ARG		189	-12.		32.644	63.200	1.00	42.01
497	CB	ARG		189	-11.		32.682	61.695	1.00	42.31
498	CG	ARG		189	-11.		31.477	61.229	1.00	44.33
499	CD	ARG		189	-9.		31.267	61.898	1.00	46.81
500	NE	ARG		189		128	30.280	61.109	1.00	54.20
500	7417	TILL	21	100	٥.	120	50.200	01.100	1.00	J4.20

FIGURE 3J

A	В	C	D	E	F	G	H	I	J
501	CZ	ARG			-9.335	28.979	61.187	1.00	56.68
502	NH1	ARG		189	-8.643	28.153	60.419	1.00	58.82
503	NH2			189	-10.230	28.496	62.049	1.00	57.84
504	C	ARG	Α	189	-12.809	34.010	63.580	1.00	41.15
505	0	ARG	Α	189	-13.554	34.620	62.819	1.00	41.64
506	N	HIS	Α	190	-12.402	34.506	64.739	1.00	40.04
507	CA	HIS	Α	190	-12.901	35.775	65.194	1.00	38.65
508	CB	HIS	Α	190	-14.316	35.605	65.760	1.00	38.81
509	CG	HIS	Α	190	-14.925	36.886	66.202	1.00	39.63
510	ND1	HIS	Α	190	-15.866	37.557	65.454	1.00	40.19
511	CE1	HIS	Α	190	-16.189	38.680	66.071	1.00	37.93
512	NE2	HIS	Α	190	-15.486	38.762	67.184	1.00	36.58
513	CD2	HIS	Α	190	-14.671	37.664	67.284	1.00	33.70
514	C	HIS	Α	190	-11.906	36.363	66.185	1.00	37.98
515	0	HIS	Α	190	-11.329	35.649	66.986	1.00	38.30
516	N	PRO	Α	191	-11.640	37.657	66.113	1.00	38.45
517	CA	PRO	Α	191	-10.581	38.239	66.953	1.00	36.82
518	CB	PRO	Α	191	-10.615	39.701	66.553	1.00	37.97
519	CG	PRO	Α	191	-12.033	39.881	66.066	1.00	38.87
520	CD	PRO	Α	191	-12.253	38.668	65.234	1.00	38.97
521	С	PRO	Α	191	-10.903	38.055	68.457	1.00	35.66
522	0	PRO	Α	191	-9.992	38.127	69.276	1.00	34.96
523	N	ASN	Α	192	-12.158	37.814	68.804	1.00	34.30
524	CA	ASN	Α	192	-12.523	37.581	70.217	1.00	33.52
525	CB	ASN	Α	192	-13.612	38.556	70.663	1.00	32.97
526	CG	ASN	Α	192	-13.207	40.027	70.497	1.00	35.71
527	OD1	ASN	Α	192	-12.286	40.503	71.178	1.00	35.61
528	ND2	ASN	Α	192	-13.823	40.714	69.556	1.00	31.27
529	С	ASN		192	-12.871	36.123	70.646	1.00	32.20
530	0	ASN		192	-13.603	35.887	71.624	1.00	31.19
531	N	ILE		193	-12.368	35.159	69.890	1.00	30.72
532	CA	ILE		193	-12.535	33.743	70.202	1.00	31.30
533	CB	ILE			-13.428	33.071	69.151	1.00	31.25
534	CG1	ILE	Α	193	-14.862	33.600	69.252	1.00	32.94
535	CD1		Α	193	-15.777	33.149	68.134	1.00	36.50
536	CG2		А	193	-13.371	31.550	69.293	1.00	29.33
537	С	ILE		193	-11.166	33.124	70.102	1.00	30.85
538	0	ILE		193	-10.472	33.376	69.121	1.00	31.20
539	N	LEU		194	-10.764	32.311	71.085	1.00	29.48
540	CA	LEU		194	-9.497	31.652	71.065	1.00	30.26
541	CB	LEU	Α	194	-9.165	31.043	72.422	1.00	28.89
542	CG	LEU		194	-7.685	30.760	72.565	1.00	31.38
543	CD1	LEU		194	-6.957	32.083	72.928	1.00	27.79
544	CD2	LEU		194	-7.565	29.741	73.655	1.00	30.09
545	C	LEU		194	-9.417	30.580	69.984	1.00	30.59
546	Ö	LEU		194	-10.224	29.651	69.930	1.00	31.64
547	N	ARG		195	-8.411	30.745	69.139	1.00	31.20
548	CA	ARG		195	-8.121	29.904	68.003	1.00	32.25
549	CB	ARG		195	-7.026	30.648	67.258	1.00	33.95
550	CG	ARG		195	-6.742	30.234	65.886	1.00	42.54
551	CD	ARG			-7.805	30.522	64.863		46.96
JJI	CD	und	12	123	-7.803	JU.JZZ	04.003	1.00	40.00

FIGURE 3K

A	В	C	D	Ε	F	G	H	I	J
552	NE	ARG	Α	195	-7.275	29.900	63.663	1.00	52.66
553	CZ	ARG		195	-6.358	30.480	62.912	1.00	56.14
554	NH1			195	-5.941	31.694	63.224	1.00	56.04
555		ARG			-5.861	29.867	61.844		60.45
556	C	ARG		195	-7.580	28.611	68.529	1.00	30.98
557	0	ARG			-6.771	28.614	69.450	1.00	28.95
558	N	LEU		196	-8.015	27.509	67.984	1.00	31.25
559	CA	LEU			-7.440	26.226	68.277	1.00	31.50
560	CB	LEU			-8.517	25.265	68.720	1.00	32.30
561	CG	LEU			-8.057	23.203	69.131	1.00	33.64
562	CD1	LEU			-9.058	23.370	70.151	1.00	36.24
563	CD2	LEU			-8.117	23.052	67.904	1.00	34.95
564	CDZ	LEU			-6.795	25.867	66.932	1.00	35.11
565	0	LEU			-7.445	25.957		1.00	34.69
566	N	TYR		197	-5.509	25.518	65.875 66.972	1.00	36.02
567	CA	TYR		197	-4.765	25.276	65.763	1.00	37.91
		TYR		197	-3.331	25.747	65.950	1.00	39.49
568	CB							1.00	
569 570	CG	TYR			-3.243 -2.704	27.233 27.782	66.128	1.00	40.35
571	CD1 CE1	TYR			-2.704	29.122	67.278 67.439	1.00	43.54
572					-3.072	29.122		1.00	44.37
573	CZ OH	TYR			-2.949	31.310	66.451 66.604	1.00	44.37
574	CE2	TYR			-3.603	29.455	65.296	1.00	45.10
575	CD2	TYR			-3.697	28.087			44.72
576	C DZ	TYR		197	-4.762	23.826	65.139 65.380	1.00	38.77
577	0	TYR		197	-4.536	23.490	64.216	1.00	39.64
578	N	GLY			-4.976	22.955	66.351	1.00	37.60
579	CA	GLY			-5.013	21.553	66.019	1.00	38.52
580	CA	GLY			-4.785	20.771	67.265	1.00	38.86
581	0	GLY			-4.900	21.311	68.409	1.00	36.64
582	N	TYR			-4.428	19.511	67.066	1.00	38.68
583	CA	TYR			-4.334	18.597	68.185	1.00	40.56
584	CB	TYR			-5.731	18.163	68.637	1.00	39.96
585	CG	TYR			-6.334	17.067	67.753	1.00	44.40
586	CD1	TYR			-7.074	17.385	66.618	1.00	44.98
587	CE1	TYR		199	-7.626	16.382	65.807	1.00	48.78
588	CZ	TYR		199	-7.420	15.058	66.132	1.00	50.76
589	OH	TYR			-7.947	14.040	65.357	1.00	58.47
590	CE2	TYR			-6.697	14.722	67.244	1.00	51.67
591	CD2	TYR			-6.160	15.736	68.060	1.00	46.05
592	C	TYR			-3.517	17.369	67.877	1.00	40.55
593	Ö	TYR		199	-3.291	17.055	66.728	1.00	40.45
594	N	PHE			-3.066	16.670	68.911	1.00	40.86
595	CA	PHE			-2.416	15.411	68.656	1.00	42.07
596	CB	PHE			-0.963	15.636	68.198	1.00	41.03
597	CG	PHE			-0.122	16.422	69.173	1.00	44.63
598	CD1	PHE			0.713	15.760	70.035	1.00	42.87
599	CE1	PHE			1.515	16.436	70.934	1.00	44.73
600	CZ	PHE			1.477	17.801	71.010	1.00	43.50
601	CE2	PHE			0.655	18.492	70.162	1.00	43.78
602		PHE			-0.191	17.817	69.254		43.04
			-						

FIGURE 3L

A	В	С	D	E	F	G	Н	I	J
603	C	PHE	Α	200	-2.610	14.522	69.888	1.00	42.82
604	0	PHE	Α	200	-3.188	14.961	70.897	1.00	39.88
605	N	HIS	Α	201	-2.268	13.251	69.770	1.00	44.66
606	CA	HIS	Α	201	-2.394	12.350	70.911	1.00	48.80
607	CB	HIS	Α	201	-3.807	11.739	70.991	1.00	49.16
608	CG	HIS	Α	201	-4.132	10.793	69.870	1.00	53.25
609	ND1	HIS	Α	201	-3.940	9.429	69.956	1.00	57.68
610	CE1	HIS	Α		-4.339	8.855	68.832	1.00	58.86
611	NE2	HIS	Α	201	-4.794	9.797	68.024	1.00	58.83
612	CD2	HIS			-4.676	11.018	68.650	1.00	57.09
613	C			201	-1.323	11.281	70.980	1.00	49.89
614	0		Α		-0.807	10.810	69.960	1.00	50.59
615	N	ASP		202	-0.983	10.943	72.219	1.00	52.70
616	CA	ASP		202	-0.084	9.828	72.492	1.00	53.99
617	CB		Α	202	1.241	10.287	73.079	1.00	54.12
618	CG		Α	202	1.098	10.887	74.444	1.00	55.69
619	OD1	ASP	Α	202	0.064	10.619	75.099	1.00	54.93
620	OD2	ASP			2.000	11.609	74.943	1.00	54.23
621	С	ASP		202	-0.819	8.790	73.330	1.00	54.16
622	0			202	-2.064	8.730	73.308	1.00	54.26
623 624	N	ALA		203	-0.084 -0.738	7.976 6.843	74.067 74.732		54.51
625	CA CB			203	0.314	5.869	75.285	1.00	54.56 54.78
626	C			203	-1.716	7.242	75.824	1.00	54.14
627	0	ALA		203	-2.869	6.753	75.824	1.00	54.14
628	N	THR		204	-1.254	8.141	76.681	1.00	52.74
629	CA	THR		204	-2.040	8.535	77.833	1.00	51.77
630	CB	THR		204	-1.114	8.467	79.073	1.00	52.77
631	OG1			204	-1.821	8.827	80.286	1.00	56.55
632	CG2	THR			-0.003	9.483	78.940	1.00	51.61
633	С	THR	Α	204	-2.689	9.929	77.704	1.00	50.02
634	0	THR	Α	204	-3.546	10.290	78.496	1.00	48.39
635	N	ARG	Α	205	-2.312	10.702	76.693	1.00	48.75
636	CA	ARG	Α	205	-2.797	12.093	76.643	1.00	47.39
637	CB	ARG	Α	205	-1.740	13.047	77.192	1.00	47.22
638	CG	ARG	Α	205	-1.295	12.746	78.573	1.00	50.14
639	CD	ARG			0.224	12.732	78.698	1.00	59.09
640	NE	ARG			0.805	13.946	79.262	1.00	65.81
641	CZ			205	2.118	14.116	79.455	1.00	71.17
642	NH1	ARG			2.587	15.256	79.974	1.00	73.74
643	NH2	ARG			2.968	13.142	79.123	1.00	72.85
644	C	ARG			-3.228	12.598	75.293	1.00	44.76
645	0	ARG			-2.831	12.070	74.258	1.00	44.49
646	N	VAL		206	-4.119	13.582	75.354	1.00	42.03
647	CA	VAL		206	-4.578	14.339	74.206	1.00	40.02
648	CB		A	206	-6.136	14.273	74.061	1.00	40.51
649 650	CG1 CG2	VAL		206 206	-6.638 -6.580	15.182 12.851	72.954 73.737	1.00	41.85
651	C	VAL		206	-4.039	15.785	74.414	1.00	38.80
652	0	VAL		206	-3.996	16.298	75.539	1.00	38.31
653	N			207	-3.593	16.409	73.339	1.00	37.44
654	CA			207	-2.976	17.737	73.430	1.00	38.03

FIGURE 3M

A	В	С	D	E	F	G	Н	1	J
655	CB	TYR	Α	207	-1.549	17.670	72.968	1.00	36.40
656	CG	TYR	Α	207	-0.688	16.778	73.766	1.00	39.00
657	CD1	TYR	Α	207	-0.010	17.249	74.881	1.00	39.70
658	CE1	TYR	Α	207	0.818	16.417	75.590	1.00	44.38
659	CZ	TYR			0.948	15.092	75.187	1.00	45.91
660	OH	TYR		207	1.734	14.246	75.900	1.00	50.45
661	CE2	TYR			0.290	14.609	74.090	1.00	43.62
662	CD2	TYR			-0.539	15.439	73.398	1.00	40.40
663	C	TYR			-3.595	18.728	72.511	1.00	37.21
664	0	TYR			-3.384	18.643	71.286	1.00	39.25
665	N	LEU			-4.323	19.685	73.049	1.00	35.21
666 667	CA CB	LEU			-4.858 -6.177	20.693	72.172 72.710	1.00	32.76
668	CG	LEU	A	208	-7.403	20.429	72.710	1.00	36.54
669	CD1	LEU	A	208	-7.148	18.880	72.249	1.00	39.94
670	CD2	LEU	A	208	-8.584	20.792	73.169	1.00	34.97
671	C	LEU		208	-3.851	21.827	71.975	1.00	31.94
672	Ö	LEU		208	-3.292	22.378	72.960	1.00	31.89
673	N	ILE	A	209	-3.605	22.175	70.710	1.00	27.64
674	CA	ILE			-2.719	23.286	70.374	1.00	29.03
675	CB	ILE	Α	209	-2.034	23.047	69.043	1.00	29.46
676	CG1	ILE			-1.424	21.632	68.983	1.00	33.03
677	CD1	ILE	Α	209	-0.629	21.353	67.616	1.00	36.54
678	CG2	ILE	Α	209	-0.996	24.092	68.833	1.00	27.57
679	C	ILE	Α	209	-3.518	24.572	70.249	1.00	29.27
680	0	ILE	Α	209	-4.206	24.763	69.258	1.00	30.08
681	N	LEU	Α	210	-3.372	25.462	71.226	1.00	27.89
682	CA	LEU		210	-4.143	26.671	71.304	1.00	28.36
683	CB	LEU	Α	210	-4.768	26.757	72.729	1.00	26.97
684	CG	LEU			-5.603	25.569	73.209	1.00	31.79
685	CD1	LEU			-6.165	25.926	74.613	1.00	31.27
686	CD2	LEU			-6.798	25.282	72.204	1.00	34.08
687 688	C	LEU		210	-3.346 -2.177	27.967 28.060	71.066 71.382	1.00	26.61
689	O N	LEU	A	211	-3.994	28.972	70.520	1.00	29.15
690	CA	GLU		211	-3.501	30.350	70.520	1.00	29.81
691	CB	GLU	A	211	-4.498	31.350	70.021	1.00	31.22
692	CG	GLU			-3.984	32.779	70.020	1.00	35.70
693	CD	GLU		211	-5.147	33.799	70.050	1.00	39.08
694	OE1	GLU			-4.932	34.950	70.489	1.00	43.39
695	OE2	GLU			-6.288	33.455	69.653	1.00	38.36
696	C	GLU		211	-3.161	30.663	72.128	1.00	29.58
697	o	GLU			-3.948	30.404	73.014	1.00	28.54
698	N	TYR	Α	212	-1.957	31.153	72.381	1.00	28.23
699	CA	TYR	Α	212	-1.550	31.606	73.725	1.00	28.20
700	CB	TYR		212	-0.028	31.697	73.739	1.00	28.08
701	CG	TYR		212	0.592	32.494	74.874	1.00	29.44
702	CD1	TYR		212	1.521	33.489	74.601	1.00	30.49
703	CE1	TYR			2.131	34.197	75.639	1.00	36.30
704	CZ	TYR			1.773	33.945	76.903	1.00	33.49
705	OH	TYR	Α	212	2.383	34.655	77.887	1.00	37.20

FIGURE 3N

A	В	С	D	E	F	G	Н	I	J
706	CE2	TYR	Α	212	0.80	2 32.97	7 77.225	1.00	33.16
707	CD2	TYR	Α	212	0.23	4 32.25	8 76.188	1.00	28.40
708	C	TYR	Α	212	-2.18	3 33.02	2 74.034	1 1.00	28.48
709	0	TYR	Α	212	-2.08	9 33.92	4 73.211	1.00	27.53
710	N	ALA	Α	213	-2.83	6 33.15	6 75.205	1.00	28.23
711	CA	ALA	Α	213	-3.43	1 34.42	4 75.650	1.00	30.33
712	CB	ALA	Α	213	-4.88				28.94
713	С	ALA	Α	213	-2.55				30.02
714	0	ALA			-2.63				31.02
715	N	PRO			-1.72				31.54
716	CA	PRO			-0.63				32.57
717	CB	PRO			0.21				32.48
718	CG	PRO			-0.49				35.80
719	CD	PRO			-1.85				30.79
720	С	PRO			-1.07				34.06
721	0	PRO		214	-0.40				35.53
722	N	LEU			-2.18				33.98
723	CA	LEU			-2.64				36.04
724	CB	LEU		215	-3.34				34.70
725	CG	LEU			-2.39				36.83
726 727	CD1 CD2	LEU			-1.15 -3.18				35.83
728	C D2	LEU			-3.10				35.81
729	0			215	-4.12				35.82
730	N	GLY		216	-3.60				35.32
731	CA	GLY		216	-4.32				34.32
732	C	GLY			-5.84				32.64
733	Ö	GLY			-6.42				32.48
734	N	THR			-6.50				31.56
735	CA	THR			-7.96				31.29
736	CB	THR			-8.51				32.13
737	OG1	THR			-8.08				30.67
738	CG2	THR			-7.97				31.12
739	C	THR	Α	217	-8.61	3 36.35	5 83.020	1.00	31.68
740	0	THR	Α	217	-8.04	1 37.06	9 83.856	1.00	28.84
741	N	VAL	Α	218	-9.88	1 36.49	8 82.686	1.00	30.86
742	CA	VAL	Α	218	-10.69	4 37.52	8 83.283	1.00	32.14
743	CB	VAL	Α	218	-11.95	3 37.67	5 82.526	1.00	33.13
744	CG1	VAL			-12.97				35.75
745	CG2	VAL			-11.61				31.98
746	C	VAL			-10.92				32.06
747	0	VAL			-11.03				32.00
748	N	TYR			-10.95				32.11
749	CA	TYR			-11.06				33.66
750	CB	TYR			-11.04				33.98
751	CG	TYR		219	-11.11				35.91
752	CD1	TYR		219	-12.33				38.53
753	CE1	TYR			-12.41				46.18
754	CZ	TYR			-11.23				47.58
755	OH	TYR			-11.32				53.35
756	CE2	TYR	А	∠19	-10.00	1 32.45	1 89.785	1.00	42.92

FIGURE 30

A	В	С	D	E	F	G	H	1	J
757	CD2	TYR	Α	219	-9.954	32.999	88.517	1.00	37.24
758	C	TYR	Α	219	-9.883	35.936	87.269	1.00	33.62
759	o	TYR			-10.105	36.423	88.379		33.27
760	N	ARG	Α	220	-8.703	35.924	86.725		
761	CA	ARG	Α	220	-7.506	36.322	87.508	1.00	36.06
762	CB	ARG	Α	220	-6.243	35.827	86.810	1.00	37.28
763	CG	ARG			-5.058	35.372	87.750	1.00	
764	CD	ARG	Α	220	-3.665	35.138	87.075	1.00	53.39
765	NE	ARG	Α	220	-3.131	36.401	86.587	1.00	57.56
766	CZ	ARG	Α	220	-3.067	36.736	85.300	1.00	63.45
767	NH1	ARG	Α	220	-2.583	37.921	84.937	1.00	62.86
768	NH2	ARG	Α	220	-3.473	35.882	84.365	1.00	65.24
769	C	ARG	Α	220	-7.561	37.846	87.621	1.00	35.84
770	0	ARG	Α	220	-7.328	38.467	88.683	1.00	34.61
771	N	GLU	Α	221	-7.928	38.427	86.490	1.00	35.98
772	CA	GLU	Α	221	-8.145	39.852	86.355	1.00	38.35
773	CB	GLU	Α	221	-8.573	40.154	84.930	1.00	39.07
774	CG	GLU	Α	221	-8.452	41.597	84.521	1.00	47.19
775	CD	GLU			-7.205	42.221	85.080	1.00	57.25
776	OE1	GLU			-6.259	42.459	84.291	1.00	60.27
777	OE2	GLU			-7.178	42.474	86.314	1.00	
778	C	GLU			-9.149	40.339	87.416	1.00	38.74
779	0			221	-8.832	41.307	88.117		38.67
780	N			222	-10.296	39.663	87.575	1.00	
781	CA			222	-11.188	40.011	88.668		
782	CB	LEU			-12.513	39.256	88.615	1.00	40.21
783	CG	LEU			-13.754	39.901	88.040	1.00	44.66
784	CD1	LEU			-13.892	41.386	88.378	1.00	
785	CD2	LEU			-13.856	39.644	86.553	1.00	
786	C	LEU			-10.654	39.766	90.079		40.79
787	0			222	-10.981	40.510	91.025	1.00	
788	N			223	-9.904	38.712	90.272		40.08
789	CA	GLN			-9.456	38.509	91.612		43.39
790	CB	GLN			-9.120	37.025	91.889	1.00	
791	CG			223	-7.754	36.535	91.538		49.87
792	CD	GLN			-7.627	34.996	91.712	1.00	
793	OE1	GLN			-6.942	34.309	90.918	1.00	58.11
794	NE2	GLN			-8.286	34.460	92.747		58.77
795 796	C	GLN			-8.380 -8.307	39.560 39.976	91.978 93.113	1.00	
797	0			223	-8.307 -7.673				43.64
798	N	LYS		224	-6.690	40.083 41.126	90.988	1.00	42.20
799	CA CB			224	-5.815	41.126	89.985		42.99
800	CG			224	-4.818	42,422	90.066	1.00	
801	CD	LYS		224	-4.028	42.585	88.762	1.00	
802	CE	LYS			-4.857	43.218	87.650		
803	NZ	LYS			-4.028	43.546	86.442		60.62
804	C	LYS			-7.356	42.461	91.560	1.00	43.04
805	0	LYS			-7.042	43.032	92.599	1.00	42.77
806	N	LEU			-8.297	42.913	90.732		40.83
807	CA	LEU			-9.019	44.181	90.897		41.08

FIGURE 3P

A	В	С	D	Е	F	G	Н	1	J
808	CB	LEU	А	225	-9.501	44.691	89.533	1.00	39.93
809	CG	LEU	Α	225	-8.469	45.241	88.540	1.00	43.97
810	CD1	LEU	Α	225	-9.133	45.930	87.345	1.00	46.75
811	CD2	LEU	Α	225	-7.332	46.154	89.189	1.00	43.17
812	C	LEU	Α	225	-10.254	44.157	91.818	1.00	40.68
813	0	LEU	Α	225	-10.784	45.218	92.182	1.00	40.10
814	N			226	-10.732	42.961	92.147	1.00	40.56
815	CA			226	-11.977	42.780	92.913	1.00	41.73
816	CB			226	-11.943	43.579	94.225	1.00	43.22
817	OG			226	-12.999	43.112	95.048	1.00	50.73
818	C			226	-13.295	43.050	92.126	1.00	40.15
819	0	SER			-14.238	42.256	92.215	1.00	40.02
820	N	LYS			-13.373	44.163	91.397	1.00	38.66
821	CA	LYS			-14.500	44.424	90.506	1.00	38.28
822	CB			227	-15.744	44.876	91.241	1.00	39.83
823 824	CG		Α		-15.527 -16.763	46.112	92.107 92.964	1.00	43.19
825	CD	LYS		227	-17.009	46.395 47.898	93.037	1.00	47.23 50.59
826	NZ	LYS			-15.847	48.527	93.755	1.00	50.07
827	C	LYS			-14.057	45.437	89.453	1.00	37.32
828	0			227	-13.032	46.114	89.637	1.00	35.43
829	N			228	-14.784	45.541	88.339	1.00	34.98
830	CA			228	-14.287	46.384	87.241	1.00	34.36
831	CB	PHE			-14.483	45.686	85.908	1.00	32.60
832	CG			228	-13.706	44.403	85.761	1.00	32.22
833	CD1			228	-12.556	44.214	86.480	1.00	30.96
834	CE1			228	-11.797	43.063	86.350	1.00	34.49
835	CZ	PHE	Α		-12.178	42.076	85.495	1.00	33.23
836	CE2	PHE	Α	228	-13.374	42.246	84.752	1.00	34.03
837	CD2	PHE	Α	228	-14.105	43.409	84.862	1.00	33.41
838	C	PHE	Α	228	-15.057	47.675	87.146	1.00	35.43
839	0	PHE	Α	228	-16.228	47.733	87.549	1.00	34.99
840	N	ASP			-14.441	48.714	86.591	1.00	36.24
841	CA	ASP			-15.233	49.943	86.453	1.00	38.49
842	CB			229	-14.302	51.205	86.331	1.00	39.70
843	CG	ASP			-13.484	51.241	85.072	1.00	44.65
844	OD1	ASP			-13.729	50.465	84.121	1.00	47.75
845	OD2	ASP			-12.527	52.046	84.948	1.00	52.81
846	С	ASP			-16.211	49.721	85.300	1.00	37.35
847	0	ASP			-16.187	48.669	84.633	1.00	35.10
848	N	GLU			-17.038	50.715	85.027	1.00	37.87
849 850	CA	GLU			-18.077	50.513	84.040	1.00	37.66
851	CB CG	GLU			-19.054 -19.840	51.668 51.650	84.115 85.412	1.00	39.25 42.58
852	CD	GLU	A	230	-21.045	52.566	85.320	1.00	42.56
853	OE1	GLU			-21.045	52.129	85.629	1.00	52.06
854	OE2	GLU		230	-20.868	53.740	84.896	1.00	52.95
855	C	GLU		230	-17.483	50.440	82.659	1.00	36.98
856	0	GLU			-18.015	49.782	81.767	1.00	34.19
857	N	GLN			-16.382	51.159	82.461	1.00	36.82
858	CA	GLN			-15.764	51.174	81.152	1.00	36.74

FIGURE 3Q

A	В	С	D	E	F	G	H	I	J
859	CB	GLN	Α	231	-14.587	52.171	81.128	1.00	37.55
860	CG	GLN			-14.995	53.671	81.393	1.00	43.18
861	CD	GLN			-16.011	53.956	82.522	1.00	46.32
862	OE1	GLN	Α	231	-15.731	53.743	83.729	1.00	42.61
863	NE2	GLN	Α	231	-17.181	54.488	82.121	1.00	47.58
864	С	GLN	Α	231	-15.212	49.784	80.817	1.00	35.85
865	0	GLN	Α	231	-15.382	49.294	79.724	1.00	36.28
866	N	ARG	Α	232	-14.495	49.186	81.746	1.00	33.62
867	CA	ARG	Α	232	-13.858	47.928	81.426	1.00	33.95
868	CB	ARG	Α		-12.832	47.530	82.509	1.00	33.54
869	CG	ARG			-12.260	46.109	82.347	1.00	36.13
870	CD	ARG			-11.433	45.610	83.520	1.00	40.91
871	NE	ARG			-10.425	46.602	83.868	1.00	49.70
872	CZ	ARG			-9.221	46.706	83.323	1.00	52.36
873	NH1	ARG			-8.817	45.862	82.371	1.00	53.98
874	NH2	ARG			-8.409	47.659	83.757	1.00	55.77
875	С	ARG			-14.931	46.853	81.238	1.00	31.99
876	0	ARG			-14.813	46.023	80.341	1.00	31.18
877	N	THR			-15.971	46.890	82.072	1.00	30.75
878 879	CA	THR			-17.071	45.931	82.002	1.00	30.48
880	CB OG1	THR			-18.080 -17.464	46.242 45.953	83.085 84.337	1.00	31.41 28.31
881	CG2	THR			-19.358	45.267	82.986	1.00	28.26
882	C	THR			-17.783	46.052	80.670	1.00	30.81
883	0	THR			-17.937	45.050	79.937		29.48
884	N	ALA			-18.283	47.261	80.402	1.00	30.12
885	CA	ALA			-18.959	47.533	79.118	1.00	30.91
886	CB	ALA			-19.319	48.998	78.963	1.00	29.68
887	C	ALA			-18.104	47.102	77.946	1.00	30.58
888	ō	ALA			-18.611	46.555	76.947	1.00	31.37
889	N	THR			-16.815	47.389	78.028	1.00	30.80
890	CA	THR			-15.928	46.948	76.953	1.00	32.35
891	CB	THR	Α	235	-14.533	47.546	77.129	1.00	32.78
892	OG1	THR	Α	235	-14.654	48.951	77.006	1.00	34.77
893	CG2	THR	Α	235	-13.580	47.153	75.967	1.00	34.42
894	C	THR	Α	235	-15.860	45.400	76.799	1.00	32.27
895	0	THR			-16.000	44.850	75.656	1.00	31.74
896	N			236	-15.711	44.693	77.914	1.00	30.81
897	CA			236	-15.676	43.199	77.861	1.00	29.77
898	CB	TYR			-15.384	42.639	79.250	1.00	29.80
899	CG			236	-13.950	42.738	79.720	1.00	32.58
900	CD1	TYR			-12.913	42.926	78.818	1.00	33.58
901	CE1	TYR			-11.617	42.996	79.243	1.00	36.97
902	CZ	TYR			-11.324	42.872	80.601	1.00	36.77
903	OH	TYR			-10.025	42.971	81.016	1.00	37.51
904	CE2	TYR			-12.330	42.686	81.516	1.00	35.78
905	CD2	TYR			-13.643	42.634	81.065	1.00	36.22
906 907	C			236 236	-17.042 -17.103	42.628 41.680	77.377 76.632	1.00	29.01
907	N			237	-17.103	43.236	77.814	1.00	30.01
909	CA	ILE			-19.472	42.788	77.378	1.00	30.81

FIGURE 3R

A	В	С	D	E		F		G		H	I	J
910	СВ	ILE	Α	237	-2	0.591	43	.548	78	3.061	1.00	29.26
911	CG1	ILE	Α	237	-2	0.580	43	.141	79	.541	1.00	31.33
912	CD1	ILE	Α	237	-2	0.607	41	.494	79	.786	1.00	32.72
913	CG2	ILE	Α	237	-2	1.938	43	.089	70	7.553	1.00	30.76
914	C	ILE	Α	237	- 3	9.524		.975	75	.874	1.00	30.97
915	0	ILE	Α	237	-2	0.024	42	.110	75	.165	1.00	28.59
916	N	THR	Α	238	-1	9.071	44	.126	75	.413	1.00	29.66
917	CA	THR	Α	238	-1	9.074	44	.331	73	3.936	1.00	31.58
918	CB	THR	Α	238	-1	8.483	45	.699	73	3.600	1.00	30.71
919	OG1	THR	Α	238	-1	9.345	46	.681	74	1.169	1.00	33.26
920	CG2	THR				8.547		.948		2.092	1.00	
921	C	THR	Α	238		8.279	43	.281		3.177	1.00	
922	0	THR				8.744		.785		2.179	1.00	
923	N	GLU				7.037		.029		3.578	1.00	
924	CA	GLU				6.252		.972		2.973	1.00	
925	CB	GLU				4.875		.829		3.619	1.00	
926	CG	GLU				4.045		.126		3.458	1.00	
927	CD	GLU				2.704		.109		1.200	1.00	
928	OE1	GLU				1.654		.089		3.518	1.00	
929	OE2	GLU				.2.655		.120		.451	1.00	
930	C	GLU				6.947		.625		.977	1.00	
931	0	GLU				6.890		.912		2.000	1.00	
932	N	LEU				7.585		.307		1.093	1.00	
933	CA	LEU				8.252		.033		1.293	1.00	
934	CB	LEU				8.793		.941		.749	1.00	
935	CG	LEU				7.918		.368		.879	1.00	
936	CD1	LEU				7.987		.156		3.226	1.00	
937	CD2	LEU				8.427		.978		7.180	1.00	
938	C	LEU				9.433		.992		3.363	1.00	
939 940	O N	LEU				9.674		.997		2.730	1.00	
941	CA	ALA				1.385		.079		2.470	1.00	
941	CB	ALA				2.161		.336		2.673	1.00	
943	C	ALA				21.046		.875).996	1.00	
944	Ö	ALA				1.803		.233		.268	1.00	
945	N	ASN				9.946		.476		.547	1.00	
946	CA	ASN				9.501		301		176	1.00	
947	CB	ASN				8.342		.225		3.806	1.00	
948	CG	ASN				8.735		.668		3.801	1.00	
949	OD1	ASN				9.820		.009		3.356	1.00	
950	ND2	ASN				7.838		.531		270	1.00	
951	C	ASN				9.045		.878		3.944	1.00	
952	0	ASN				9.384		.322		7.926	1.00	
953	N	ALA				8.284		.287		.871	1.00	
954	CA	ALA	Α	243	-1	7.846	36	.899	69	.686	1.00	33.50
955	CB	ALA	Α	243	-1	6.883	36	.413	70	.821	1.00	32.46
956	C	ALA	Α	243		9.100	36	.026	69	.596	1.00	33.00
957	0	ALA	Α	243	- 1	9.170	35	.121	68	3.775	1.00	34.04
958	N	LEU				0.063		.281		.460	1.00	
959	CA	LEU				1.290		.495		.486	1.00	
960	CB	LEU	Α	244	-2	22.109	35	.794	71	1.761	1.00	32.72

FIGURE 3S

A	В	С	D	E	F	G	H	1	J
961	CG	LEU	Α	244	-21.487	35.248	73.091	1.00	33.90
962	CD1	LEU	Α	244	-22.375	35.636	74.211	1.00	34.58
963	CD2	LEU	Α	244	-21.346	33.731	73.053	1.00	36.04
964	C	LEU	Α	244	-22.155	35.710	69.239	1.00	35.07
965	0	LEU	Α	244	-22.795	34.770	68.771	1.00	35.54
966	N	SER	Α	245	-22.205	36.935	68.736	1.00	36.14
967	CA	SER	Α	245	-22.968	37.144	67.497	1.00	37.32
968	CB	SER	Α	245	-22.881	38.566	66.993	1.00	36.71
969	OG	SER	Α	245	-23.518	39.430	67.885	1.00	40.23
970	C	SER	Α	245	-22.396	36.244	66.430	1.00	37.77
971	0	SER	Α	245	-23.168	35.561	65.712	1.00	39.78
972	N	TYR	Α	246	-21.062	36.236	66.324	1.00	36.62
973	CA	TYR			-20.388	35.397	65.334	1.00	36.75
974	CB	TYR	Α	246	-18.867	35.666	65.303	1.00	35.63
975	CG	TYR	Α	246	-18.040	34.768	64.415	1.00	36.74
976	CD1	TYR			-17.752	35.114	63.086	1.00	41.06
977	CE1	TYR			-16.991	34.283	62.293	1.00	40.63
978	CZ	TYR			-16.491	33.118	62.824	1.00	42.34
979	OH	TYR			-15.711	32.256	62.077	1.00	41.50
980	CE2	TYR			-16.782	32.766	64.151	1.00	40.05
981	CD2	TYR			-17.538	33.590	64.897	1.00	34.12
982	C	TYR			-20.730	33.925	65.554	1.00	36.80
983	0	TYR			-21.143	33.248	64.624	1.00	36.65
984	N	CYS			-20.608	33.425	66.778	1.00	36.48
985	CA	CYS			-21.015	32.049	67.085	1.00	36.90
986	CB	CYS			-20.803	31.722	68.595	1.00	37.60
987	SG	CYS			-19.067	31.666	69.093	1.00	42.84
988	С	CYS			-22.473	31.711	66.758	1.00	37.39
989	0	CYS			-22.746	30.672	66.121	1.00	37.58
990	N	HIS			-23.400	32.529	67.256	1.00	36.67
991	CA	HIS			-24.817	32.267	67.094	1.00	37.58
992	CB	HIS			-25.698	33.244	67.876	1.00	37.99
993 994	CG			248	-25.520	33.191	69.372	1.00	34.73
	ND1	HIS			-26.053	34.149	70.204	1.00	36.33
995 996	CE1 NE2	HIS	Α		-25.718 -24.957	33.886	71.452	1.00	37.79
996	CD2	HIS			-24.957	32.807 32.354	71.458	1.00	33.84
998	CDZ	HIS			-25.189	32.334	65.601	1.00	39.08
999	0	HIS			-26.098	31.629	65.132	1.00	39.68
1000	N	SER			-24.443	33.132	64.854	1.00	39.67
1000	CA	SER			-24.748	33.244	63.437	1.00	41.50
1002	CB	SER			-23.805	34.207	62.715	1.00	40.00
1003	OG	SER			-22.561	33.599	62.481	1.00	41.00
1003	C	SER			-24.644	31.857	62.870	1.00	42.73
1005	Ö	SER		249	-25.312	31.550	61.894	1.00	43.62
1006	N	LYS			-23.799	31.026	63.476	1.00	43.39
1007	CA	LYS			-23.626	29.655	63.026	1.00	44.23
1008	CB	LYS			-22.163	29.299	63.057	1.00	45.26
1009	CG	LYS			-21.329	30.154	62.111	1.00	46.88
1010	CD	LYS			-19.847	29.989	62.369	1.00	46.41
1011	CE	LYS	Α	250	-19.102	31.086	61.674	1.00	50.41

FIGURE 3T

Α	В	С	D	Е	F	G	Н	1	J
1012	NZ	LYS	Α	250	-18.101	30.510	60.721	1.00	55.71
1013	C	LYS	Α	250	-24.430	28.706	63.912	1.00	44.23
1014	0	LYS	Α	250	-24.318	27.494	63.813	1.00	44.92
1015	N	ARG	Α	251	-25.252	29.280	64.771	1.00	43.03
1016	CA	ARG	Α	251	-26.013	28.499	65.722	1.00	43.09
1017	CB	ARG	Α	251	-27.003	27.566	65.025	1.00	44.17
1018	CG	ARG	Α	251	-28.079	28.334	64.298	1.00	48.00
1019	CD	ARG	Α	251	-29.293	28.613	65.135	1.00	52.94
1020	NE	ARG			-30.316	27.613	64.935	1.00	57.46
1021	CZ	ARG			-31.409	27.504	65.694	1.00	59.77
1022	NH1				-32.301	26.573	65.421	1.00	58.50
1023		ARG			-31.617	28.329	66.721	1.00	60.29
1024	C	ARG			-25.133	27.719	66.694	1.00	40.87
1025	0	ARG			-25.579	26.725	67.287	1.00	41.62
1026	N	VAL			-23.890	28.136	66.866	1.00	38.05
1027	CA	VAL			-23.090	27.469	67.883	1.00	35.63
1028	CB	VAL			-21.605	27.579	67.574	1.00	36.71
1029	CG1	VAL			-20.757	27.253	68.833	1.00	36.16
1030 1031	CG2	VAL			-21.267	26.671 28.171	66.408	1.00	32.96
1031	C	VAL			-23.398 -23.342	29.421	69.217 69.278	1.00	35.05 34.28
1032	N	ILE			-23.751	27.394	70.238	1.00	34.28
1033	CA			253	-24.036	27.990	71.537	1.00	34.78
1034	CB	ILE		253	-25.528	27.772	72.035	1.00	36.92
1036	CG1	ILE	A	253	-26.008	26.317	72.080	1.00	34.92
1037	CD1	ILE		253	-27.473	26.046	72.506	1.00	33.07
1038	CG2			253	-26.490	28.538	71.085	1.00	39.25
1039	C			253	-22.899	27.570	72.441	1.00	32.53
1040	Ö	ILE		253	-22.459	26.397	72.378	1.00	32.33
1041	N			254	-22.352	28.508	73.234	1.00	30.81
1042	CA	HIS	Α	254	-21.118	28.158	73.987	1.00	29.80
1043	CB	HIS		254	-20.268	29.410	74.275	1.00	29.82
1044	CG	HIS	Α	254	-19.012	29.095	75.010	1.00	27.09
1045	ND1	HIS	Α	254	-19.012	28.695	76.327	1.00	28.08
1046	CE1	HIS	Α	254	-17.763	28.515	76.729	1.00	29.12
1047	NE2	HIS	Α	254	-16.960	28.776	75.712	1.00	31.85
1048	CD2	HIS		254	-17.712	29.137	74.622	1.00	26.39
1049	C	HIS		254	-21.449	27.412	75.287	1.00	29.59
1050	0	HIS		254	-20.897	26.345	75.563	1.00	28.85
1051	N	ARG			-22.405	27.957	76.024	1.00	30.83
1052	CA	ARG			-22.920	27.309	77.234	1.00	30.64
1053	CB	ARG			-23.388	25.859	76.916	1.00	30.22
1054	CG	ARG			-24.321	25.716	75.687	1.00	32.25
1055	CD			255	-25.189	24.432	75.685	1.00	31.75
1056	NE CZ	ARG ARG			-24.362	23.256	75.649 75.669	1.00	30.77
1057 1058	NH1	ARG		255	-24.820 -26.095	22.017	75.669	1.00	31.35
1058	NH1	ARG		255	-28.095	21.798	75.617	1.00	33.16
1060	C	ARG			-21.983	27.279	78.449	1.00	31.38
1061	0	ARG			-22.363	26.734	79.477	1.00	32.65
1062	N	ASP			-20.758	27.768	78.356	1.00	31.39

FIGURE 3U

A	В	С	D	E	F	G	H	I	J
1063	CA	ASP	Α	256	-19.870	27.725	79.524	1.00	31.75
1064	CB	ASP			-18.964	26.468	79.453	1.00	33.11
1065	CG	ASP	Α	256	-18.280	26.139	80.746	1.00	35.07
1066	OD1	ASP			-18.773	26.510	81.850	1.00	40.12
1067	OD2	ASP	Α	256	-17.221	25.488	80.765	1.00	36.02
1068	C	ASP	Α	256	-19.086	29.003	79.566	1.00	31.14
1069	0	ASP	Α	256	-17.867	29.025	79.770	1.00	30.07
1070	N	ILE	Α	257	-19.785	30.091	79.314	1.00	29.90
1071	CA	ILE	Α	257	-19.166	31.390	79.385	1.00	32.07
1072	CB	ILE	Α	257	-20.057	32.311	78.676	1.00	32.32
1073	CG1	ILE	Α	257	-19.935	31.982	77.143	1.00	33.96
1074	CD1			257	-21.111	32.476	76.377	1.00	40.55
1075	CG2	ILE	Α	257	-19.737	33.701	78.956	1.00	34.18
1076	C	ILE		257	-19.064	31.704	80.897	1.00	33.31
1077	0	ILE		257	-20.100	31.754	81.616	1.00	34.68
1078	N	LYS		258	-17.824	31.761	81.371	1.00	31.48
1079	CA			258	-17.519	32.187	82.750	1.00	30.84
1080	CB			258	-17.738	31.082	83.740	1.00	30.14
1081	CG			258	-16.926	29.870	83.529	1.00	34.40
1082	CD			258	-17.629	28.644	84.283	1.00	38.03
1083	CE			258	-16.742	27.431	84.270	1.00	41.53
1084	NZ			258	-17.580	26.165	84.236	1.00	42.89
1085	С			258	-16.097	32.737	82.755	1.00	30.04
1086	0	LYS		258	-15.324	32.537	81.785	1.00	26.95
1087	N	PRO			-15.775	33.505	83.792	1.00	28.33
1088	CA			259	-14.498	34.201	83.824	1.00	28.63
1089	CB			259	-14.480	34.892	85.200	1.00	27.18
1090 1091	CG			259 259	-15.974 -16.648	35.164 33.843	85.421 84.942	1.00	28.54
1091	C			259	-13.330	33.301	83.615	1.00	27.22
1093	0			259	-12.411	33.740	82.963	1.00	28.73
1094	N			260	-13.331	32.086	84.121	1.00	27.82
1095	CA			260	-12.176	31.226	83.876	1.00	28.92
1096	CB			260	-12.107	30.028	84.836	1.00	31.10
1097	CG	GLU			-13.445	29.310	84.935	1.00	35.20
1098	CD			260	-14.340	29.861	86.098	1.00	44.01
1099	OE1	GLU			-14.462	29.148	87.133	1.00	49.68
1100	OE2	GLU	Α	260	-14.908	30.985	86.003	1.00	33.54
1101	С	GLU	Α	260	-12.027	30.755	82.420	1.00	28.10
1102	0	GLU	Α	260	-10.957	30.265	82.068	1.00	29.64
1103	N	ASN	Α	261	-13.012	30.991	81.567	1.00	26.88
1104	CA	ASN	Α	261	-12.871	30.603	80.189	1.00	26.98
1105	CB	ASN	Α	261	-14.077	29.731	79.753	1.00	26.91
1106	CG	ASN	Α	261	-14.099	28.389	80.436	1.00	26.82
1107	OD1			261	-13.048	27.832	80.771	1.00	28.36
1108	ND2	ASN		261	-15.322	27.808	80.578	1.00	25.54
1109	C	ASN		261	-12.786	31.829	79.266	1.00	28.17
1110	0	ASN			-12.988	31.685	78.040	1.00	28.42
1111	N			262	-12.540	33.021	79.848	1.00	27.97
1112	CA			262	-12.454	34.254	79.091	1.00	
1113	CB	LEU	Α	262	-13.351	35.341	79.662	1.00	29.50

FIGURE 3V

A	В	С	D	E	F	G	Н	I	J
1114	CG	LEU	Α	262	-14.856	35.024	79.655	1.00	28.47
1115	CD1	LEU	Α	262	-15.646	36.167	80.215	1.00	30.27
1116	CD2	LEU	Α	262	-15.308	34.782	78.142	1.00	27.13
1117	C	LEU	Α	262	-11.011	34.681	79.268	1.00	29.16
1118	0	LEU	Α	262	-10.554	34.891	80.405	1.00	28.97
1119	N	LEU	Α	263	-10.299	34.765	78.163	1.00	26.56
1120	CA	LEU	Α	263	-8.869	34.988	78.194	1.00	28.18
1121	CB	LEU	Α	263	-8.103	33.942	77.360	1.00	26.68
1122	CG	LEU	Α	263	-8.452	32.452	77.583	1.00	29.56
1123	CD1	LEU	Α	263	-7.487	31.481	76.825	1.00	30.33
1124	CD2	LEU	Α	263	-8.272	32.171	79.060	1.00	34.69
1125	C	LEU	Α	263	-8.574	36.382	77.619	1.00	29.97
1126	0	LEU	Α	263	-9.416	37.002	76.966	1.00	29.84
1127	N	LEU	Α	264	-7.378	36.850	77.904	1.00	30.85
1128	CA	LEU			-6.951	38.182	77.486	1.00	30.74
1129	CB	LEU		264	-6.721	39.079	78.732	1.00	30.19
1130	CG	LEU			-7.965	39.287	79.626	1.00	30.14
1131	CD1	LEU		264	-7.590	39.909	81.031	1.00	32.30
1132	CD2	LEU			-9.105	40.109	78.954	1.00	31.52
1133	C	LEU			-5.737	38.121	76.554	1.00	30.62
1134	0	LEU			-4.722	37.498	76.853	1.00	29.43
1135	N	GLY			-5.901	38.736	75.390	1.00	31.75
1136	CA	GLY			-4.858	38.816	74.396	1.00	33.01
1137	С	GLY			-3.830	39.883	74.737	1.00	34.94
1138	0	GLY			-3.969	40.574	75.751	1.00	34.96
1139	N			266	-2.807	40.035	73.891	1.00	36.48
1140	CA			266	-1.722	40.978	74.178	1.00	39.30
1141	CB			266	-0.547	40.820	73.179	1.00	39.61
1142	OG			266	-1.009	40.865	71.841	1.00	45.24
1143 1144	C			266	-2.195 -1.591	42.443	74.287	1.00	39.68 41.74
1144	0			266	-3.286	43.221	73.641	1.00	39.84
1145	N CA	ALA			-3.757	44.193	73.821	1.00	40.82
1147	CB	ALA			-4.312	44.745	72.510	1.00	41.57
1148	C	ALA			-4.826	44.245	74.881	1.00	40.28
1149	0	ALA			-5.507	45.246	75.017	1.00	41.69
1150	N	GLY			-4.999	43.160	75.616	1.00	38.92
1151	CA	GLY			-6.066	43.100	76.605	1.00	39.91
1152	C	GLY			-7.440	42.772	76.035	1.00	39.16
1153	0	GLY			-8.421	42.894	76.749	1.00	39.70
1154	N	GLU			-7.525	42.328	74.781	1.00	37.55
1155	CA	GLU			-8.846	42.066	74.210	1.00	37.18
1156	CB	GLU			-8.844	42.024	72.686	1.00	36.91
1157	CG	GLU			-7.914	40.966	72,111	1.00	42.45
1158	CD	GLU			-6.497	41.495	71.931	1.00	48.18
1159	OE1	GLU			-5.789	41.696	72.951	1.00	49.56
1160	OE2	GLU	Α	269	-6.122	41.758	70.767	1.00	54.50
1161	C	GLU	Α	269	-9.323	40.711	74.736	1.00	34.23
1162	0	GLU	Α	269	-8.556	39.821	74.981	1.00	32.16
1163	N	LEU	Α	270	-10.611	40.599	74.889	1.00	33.25
1164	CA	LEU	Α	270	-11.188	39.438	75.496	1.00	33.59

FIGURE 3W

A	В	С	D	E	F	G	H	I	J
1165	CB	TEIT	70	270	-12.532	39.836	76.065	1.00	33.76
1166	CG	LEU		270	-13.339	38.735	76.759	1.00	35.55
1167	CD1			270	-14.388	39.362	77.722	1.00	38.75
1168	CD2			270	-14.078	37.912	75.720	1.00	35.40
1169				270	-11.330	38.372	74.432	1.00	33.86
	C								
1170	0			270	-11.671	38.675	73.243	1.00	34.74
1171	N	LYS		271	-11.099	37.133	74.834	1.00	31.42
1172	CA			271	-11.191	35.979	73.930	1.00	31.29
1173	CB	LYS		271	-9.795	35.492	73.555	1.00	31.80
1174	CG	LYS			-9.128	36.524	72.537	1.00	35.49
1175	CD	LYS			-7.766	36.110	72.033	1.00	38.66
1176	CE	LYS		271	-7.165	37.192	71.120	1.00	39.08
1177	NZ			271	-7.494	36.998	69.682	1.00	42.36
1178	С	LYS		271	-11.994	34.844	74.605	1.00	29.90
1179	0	LYS		271	-11.668	34.417	75.687	1.00	30.82
1180	N	ILE		272	-13.062	34.408	73.997	1.00	29.63
1181	CA	ILE		272	-13.770	33.287	74.572	1.00	31.28
1182	CB			272	-15.251	33.238	74.154	1.00	32.97
1183	CG1	ILE		272	-15.867	31.943	74.660	1.00	34.14
1184	CD1	ILE	Α	272	-17.133	32.166	75.428	1.00	41.15
1185	CG2	ILE	Α	272	-15.415	33.105	72.693	1.00	36.72
1186	C	ILE	Α	272	-12.981	32.023	74.227	1.00	29.77
1187	0	ILE	Α	272	-12.487	31.888	73.131	1.00	29.32
1188	N	ALA	Α	273	-12.833	31,121	75.199	1.00	29.03
1189	CA	ALA	Α	273	-12.072	29.905	75.040	1.00	28.02
1190	CB	ALA	Α	273	-10.720	30.027	75.796	1.00	25.93
1191	С	ALA	Α	273	-12.890	28.757	75.639	1.00	28.47
1192	0	ALA	Α	273	-14.008	28.975	76.165	1.00	29.27
1193	N	ASP	Α	274	-12.329	27.558	75.567	1.00	28.32
1194	CA	ASP	Α	274	-12.900	26.361	76.217	1.00	30.13
1195	CB	ASP	Α	274	-12.994	26.548	77.752	1.00	28.19
1196	CG	ASP	Α	274	-13.273	25.239	78.444	1.00	30.91
1197	OD1	ASP	Α	274	-13.354	25.219	79.681	1.00	27.79
1198	OD2	ASP	Α	274	-13.407	24.145	77.794	1.00	33.55
1199	С	ASP	Α	274	-14.278	25.977	75.649	1.00	29.52
1200	0	ASP	Α	274	-15.326	26.170	76.275	1.00	28.76
1201	N	PHE	Α	275	-14.288	25.489	74.427	1.00	29.79
1202	CA	PHE			-15.564	25.206	73.796	1.00	31.48
1203	CB	PHE		275	-15.508	25.464	72.250	1.00	30.13
1204	CG	PHE			-15.621	26.887	71.890	1.00	30.02
1205	CD1				-14.605	27.761	72.243	1.00	30.82
1206	CE1	PHE			-14.705	29.121	71.908	1.00	31.65
1207	CZ	PHE			-15.847	29.599	71.217	1.00	30.66
1208	CE2	PHE		275	-16.846	28.718	70.853	1.00	28.29
1209	CD2	PHE		275	-16.707	27.356	71.175	1.00	28.74
1210	C			275	-16.042	23.793	74.019	1.00	31.32
1211	Ö	PHE			-16.874	23.333	73.263	1.00	33.58
1212	N			276	-15.542	23.128	75.050	1.00	32.57
1213	CA			276	-15.980	21.764	75.409	1.00	33.27
1214	C			276	-17.470	21.591	75.718	1.00	33.63
1215	0			276	-18.005	20.503	75.585		35.45
1210	_	ОПІ	7.1	~ . 0	10.000	20.000	.0.000	1.00	55.45

FIGURE 3X

A	В	С	D	E	F	G	Н	1	J
1216	N	TRP	Α	277	-18.168	22.649	76.085	1.00	32.48
1217	CA	TRP	Α	277	-19.590	22.515	76.352	1.00	32.61
1218	CB	TRP	Α	277	-19.996	23.356	77.571	1.00	31.90
1219	CG			277	-19.872	22.560	78.827	1.00	33.69
1220	CD1			277	-18.906	22.655	79.755	1.00	35.79
1221	NE1	TRP			-19.139	21.779	80.781	1.00	39.83
1222	CE2	TRP			-20.287	21.083	80.520	1.00	39.15
	CD2							1.00	
1223 1224	CE3	TRP			-20.784 -21.976	21.563	79.295 78.795	1.00	36.18
1225	CZ3	TRP			-22.625	19.991	79.531	1.00	40.23
1226	CH2	TRP			-22.103	19.550	80.772	1.00	36.38
1227	CZ2	TRP			-20.945	20.080	81.281	1.00	39.03
1228	С			277	-20.375	22.965	75.141	1.00	31.77
1229	0	TRP			-21.575	22.921	75.138	1.00	31.92
1230	N			278	-19.701	23.425	74.102	1.00	30.59
1231	CA			278	-20.489	23.978	73.041	1.00	32.01
1232	CB			278	-19.643	24.889	72.181	1.00	32.28
1233	OG			278	-18.600	24.165	71.545	1.00	37.30
1234	C	SER	Α	278	-21.253	22.892	72.194	1.00	33.25
1235	0			278	-20.861	21.734	72.149	1.00	34.86
1236	N	VAL			-22.353	23.307	71.560	1.00	34.55
1237	CA	VAL	Α	279	-23.201	22.424	70.775	1.00	36.63
1238	CB	VAL	Α	279	-24.238	21.763	71.710	1.00	36.03
1239	CG1	VAL	Α	279	-25.173	22.788	72.273	1.00	35.73
1240	CG2	VAL	Α	279	-24.920	20.585	71.018	1.00	38.77
1241	С	VAL	Α	279	-23.873	23.260	69.702	1.00	36.61
1242	0	VAL	Α	279	-23.927	24.488	69.850	1.00	35.60
1243	N	HIS	Α	280	-24.438	22.679	68.636	1.00	37.41
1244	CA	HIS	Α	280	-25.231	23.526	67.764	1.00	37.57
1245	CB	HIS	Α	280	-25.245	22.996	66.333	1.00	39.08
1246	CG	HIS	Α	280	-23.897	23.025	65.714	1.00	39.44
1247		HIS			-23.001	21.988	65.841	1.00	45.81
1248		HIS			-21.883	22.296	65.203	1.00	45.95
1249		HIS			-22.028	23.493	64.660	1.00	46.60
1250	CD2				-23.283	23.969	64.964	1.00	45.31
1251	C	HIS			-26.590	23.569	68.343	1.00	37.33
1252	0	HIS			-27.040	22.566	68.911	1.00	37.60
1253	N	ALA			-27.212	24.737	68.237	1.00	36.55
1254	CA	ALA			-28.494	25.000	68.825	1.00	38.46
1255	CB	ALA			-28.828	26.461	68.875	1.00	37.40
1256	C	ALA			-29.597	24.175	68.213	1.00	41.55
1257	0	ALA			-29.485	23.958	67.009	1.00	41.26
1258	N			282	-30.764	24.290	68.822	1.00	41.87
1259	CA	PRO			-31.606	23.344	69.535	1.00	41.68
1260	CB			282	-32.618	22.859	68.482	1.00	42.55
	CG			282	-32.018	23.675	67.281	1.00	
1261									41.31
1262	CD			282	-31.631	25.026	67.910	1.00	44.02
1263	C			282	-30.712	22.264	70.155	1.00	40.86
1264	0			282	-30.004	21.537	69.457	1.00	40.78
1265	N			283	-30.704	22.233	71.483	1.00	38.89
1266	CA	SER	Α	283	-30.011	21.158	72.148	1.00	39.04

FIGURE 3Y

A	В	С	D	Ε	F	G	H	1	J
1267	СВ	SER	Α	283	-28.515	21.411	72.222	1.00	38.52
1268	OG			283	-27.832	20.358	72.915	1.00	40.61
1269	C			283	-30.549	20.857	73.526	1.00	39.37
1270	ō			283	-31.163	21.706	74.190	1.00	39.84
1271	N			284	-30.310	19.641	73.955	1.00	39.43
1272	CA			284	-30.584	19.299	75.314	1.00	41.76
1273	CB			284	-31.245	17.940	75.356	1.00	43.22
1274	OG			284	-32.242	17.954	76.372	1.00	47.58
1275	C			284	-29.239	19.218	75.979	1.00	42.43
1276							75.432		
	0			284	-28.205	19.677		1.00	43.18
1277	N			285	-29.226	18.626	77.161	1.00	42.91
1278	CA	ARG			-27.980	18.390	77.875	1.00	43.85
1279	CB	ARG			-27.914	19.247	79.145	1.00	43.75
1280	CG	ARG			-26.582	19.105	79.889	1.00	43.99
1281	CD			285	-26.415	20.119	81.009	1.00	45.74
1282	NE			285	-27.612	20.161	81.838	1.00	49.71
1283	CZ			285	-27.710	19.525	82.988	1.00	52.93
1284	NH1	ARG			-28.822	19.597	83.713	1.00	53.76
1285	NH2	ARG			-26.675	18.805	83.415	1.00	55.88
1286	С	ARG			-27.906	16.906	78.267	1.00	43.69
1287	0			285	-28.836	16.435	78.958	1.00	44.26
1288	N			288	-25.116	15.611	79.501	1.00	47.82
1289	CA	THR	Α	288	-23.866	15.594	80.345	1.00	48.76
1290	CB	THR	Α	288	-22.675	16.360	79.646	1.00	48.89
1291	OG1	THR	Α	288	-22.479	15.933	78.293	1.00	51.35
1292	CG2	THR	Α	288	-21.345	16.015	80.297	1.00	47.79
1293	С	THR	Α	288	-24.101	16.243	81.732	1.00	49.14
1294	0	THR	Α	288	-24.852	17.214	81.851	1.00	47.49
1295	N	LEU	Α	289	-23.443	15.702	82.757	1.00	50.43
1296	CA	LEU	Α	289	-23.441	16.283	84.118	1.00	53.20
1297	CB	LEU	Α	289	-22.802	15.267	85.056	1.00	53.63
1298	CG	LEU	Α	289	-23.766	14.793	86.121	1.00	57.03
1299	CD1	LEU	Α	289	-24.112	15.959	87.046	1.00	59.33
1300	CD2	LEU	Α	289	-25.011	14.189	85.463	1.00	60.93
1301	С	LEU	Α	289	-22.694	17.651	84.276	1.00	53.31
1302	0	LEU	Α	289	-21.619	17.817	83.725	1.00	53.60
1303	N	CYS	Α	290	-23.229	18.557	85.113	1.00	55.50
1304	CA	CYS	Α	290	-22.752	19.970	85.335	1.00	57.08
1305	CB	CYS			-23.926	20.833	85.843	1.00	57.49
1306	SG	CYS	Α	290	-25.205	21.169	84.585	1.00	64.10
1307	С	CYS			-21.426	20.313	86.110	1.00	56.52
1308	Ó			290	-20.448	19.597	85.933	1.00	57.86
1309	N	GLY			-21.379	21.417	86.898	1.00	55.52
1310	CA	GLY			-20.169	21.921	87.613	1.00	52.28
1311	C	GLY			-20.635	23.035	88.583	1.00	50.12
1312	ŏ	GLY			-21.578	22.837	89.335	1.00	49.36
1313	N			292	-20.005	24.208	88.624	1.00	47.90
1314	CA			292	-20.610	25.273	89.444	1.00	44.87
1315	CB			292	-19.672	26.461	89.703	1.00	47.07
1316	OG1			292	-20.442	27.619	90.103	1.00	47.16
1317	CG2			292	-19.180	26.950	88.383	1.00	48.62
1311	CGZ	1111	21	232	17.100	20.930	00.303	1.00	40.02

FIGURE 3Z

A	В	С	D	E	F	G	H	1	J
1318	С	THR	Α	292	-21.798	25.781	88.602	1.00	41.88
1319	0	THR	Α	292	-21.634	25.980	87.395	1.00	41.81
1320	N	LEU	Α	293	-22.964	26.018	89.200	1.00	36.57
1321	CA	LEU			-24.101	26.475	88.391	1.00	35.69
1322	CB			293	-25.398	26.116	89.074	1.00	35.41
1323				293	-26.168			1.00	
	CG					24.807	88.850		42.89
1324	CD1	LEU			-25.377	23.623	88.364	1.00	43.78
1325	CD2	LEU			-27.014	24.434	90.111	1.00	43.98
1326	C	LEU			-24.158	27.975	88.146	1.00	33.14
1327	0	LEU			-25.017	28.435	87.395	1.00	32.15
1328	N	ASP			-23.246	28.729	88.755	1.00	31.34
1329	CA	ASP			-23.362	30.191	88.780	1.00	30.17
1330	CB	ASP	Α	294	-22.072	30.788	89.362	1.00	31.41
1331	CG	ASP	Α	294	-22.096	30.775	90.875	1.00	36.52
1332	OD1	ASP	Α	294	-21.149	30.228	91.449	1.00	42.47
1333	OD2	ASP	Α	294	-23.074	31.224	91.535	1.00	39.71
1334	С	ASP	Α	294	-23.740	30.941	87.510	1.00	29.90
1335	ō	ASP			-24.404	31.966	87.568	1.00	28.82
1336	N	TYR			-23.192	30.486	86.390	1.00	
1337	CA	TYR			-23.409	31.144	85.110	1.00	29.18
1338	CB	TYR			-22.081	31.134	84.392	1.00	29.58
1339	CG			295	-21.064	31.857	85.196	1.00	28.98
1340	CD1	TYR			-20.229	31.183	86.080	1.00	33.43
1341	CE1	TYR			-19.281	31.854	86.858	1.00	35.92
1342	CZ			295	-19.257	33.216	86.782	1.00	33.99
1343	OH			295	-18.331	33.880	87.548	1.00	39.27
1344	CE2	TYR			-20.078	33.903	85.910	1.00	33.69
1345	CD2	TYR			-20.983	33.215	85.124	1.00	32.42
1346	С			295	-24.468	30.562	84.180	1.00	30.12
1347	0			295	-24.606	31.005	83.032	1.00	29.57
1348	N	LEU			-25.192	29.556	84.637	1.00	29.88
1349	CA			296	-26.160	28.872	83.753	1.00	30.57
1350	CB			296	-26.090	27.394	83.996	1.00	31.08
1351	CG			296	-24.686	26.827	83.787	1.00	36.71
1352	CD1	LEU			-24.675	25.310	84.148	1.00	38.55
1353	CD2	LEU	Α	296	-24.209	27.111	82.373	1.00	35.88
1354	C	LEU	Α	296	-27.547	29.301	84.042	1.00	30.06
1355	0	LEU	Α	296	-27.902	29.441	85.223	1.00	28.76
1356	N	PRO	Α	297	-28.346	29.432	82.969	1.00	29.59
1357	CA	PRO	Α	297	-29.752	29.814	83.035	1.00	29.63
1358	CB	PRO	Α	297	-30.105	30.142	81.563	1.00	30.10
1359	CG	PRO			-29.256	29.232	80.816	1.00	30.36
1360	CD			297	-27.902	29.176	81.578	1.00	30.37
1361	Ċ	PRO			-30.593	28.606	83.518	1.00	30.53
1362	o			297	-30.133	27.475	83.493	1.00	29.72
1363	N			298	-31.785	28.907	83.980	1.00	32.38
1364	CA			298	-32.748	27.911	84.486	1.00	35.25
1365	CB			298	-34.030	28.716	84.623	1.00	34.69
1366	CG			298	-33.555	30.121	84.897	1.00	35.48
1367	CD			298	-32.269	30.280	84.096	1.00	32.59
1368				298	-32.269	26.766			
1208	С	rko	14	296	-32.931	∠0./00	83.492	1.00	37.27

FIGURE 3AA

A	В	С	D	Е	F	G	H	1	J
1369	0	PRO	Α	298	-32.829	25.611	83.920	1.00	38.20
1370	N	GLU	Α	299	-33.089	27.056	82.197	1.00	38.20
1371	CA	GLU			-33.396	25.984	81.252		40.09
1372	CB	GLU			-33.745	26.499	79.833		39.94
1373	CG	GLU			-32.614	27.242	79.139		39.16
1374	CD	GLU			-32.578	28.754	79.410		39.82
1375	OE1	GLU			-33.124	29.242	80.436		37.57
1376	OE2	GLU			-31.980	29.467	78.564		37.07
1377	C	GLU			-32.299	24.969	81.174		41.23
1378		GLU			-32.299	23.747			
1379	0	MET			-31.075	25.468	81.097 81.248	1.00	41.06
	N								
1380	CA			300	-29.951	24.596	81.206		43.22
1381	CB	MET			-28.679	25.376	81.027		43.88
1382	CG			300	-27.499	24.515	81.020		49.44
1383	SD			300	-26.839	24.501	79.396		60.26
1384	CE	MET			-25.544	23.343	79.572	1.00	54.71
1385	С			300	-29.837	23.750	82.461		44.15
1386	0	MET			-29.682	22.512	82.356	1.00	44.33
1387	N			301	-29.864	24.362	83.638		44.85
1388	CA	ILE			-29.735	23.521	84.831	1.00	46.79
1389	CB			301	-29.657	24.332	86.111	1.00	47.71
1390	CG1	ILE			-30.818	25.308	86.276		50.37
1391	CD1	ILE	Α	301	-30.163	26.709	86.641		56.06
1392	CG2	ILE	Α	301	-28.369	25.222	86.119	1.00	46.42
1393	C	ILE	Α	301	-30.836	22.441	84.891	1.00	48.14
1394	0	ILE	Α	301	-30.538	21.258	85.093	1.00	48.00
1395	N	GLU	Α	302	-32.085	22.854	84.677	1.00	49.20
1396	CA	GLU	Α	302	-33.236	21.952	84.671	1.00	51.02
1397	CB	GLU	Α	302	-34.520	22.754	84.559	1.00	51.41
1398	CG	GLU	Α	302	-34.831	23.576	85.792	1.00	55.27
1399	CD	GLU	Α	302	-35.798	24.695	85.474	1.00	59.81
1400		GLU			-36.087	25.555	86.349		63.64
1401	OE2	GLU			-36.294	24.693	84.335		60.77
1402	Ċ	GLU			-33.242	20.937	83.540		51.10
1403	Ó	GLU			-34.179	20.143	83.434		51.91
1404	N	GLY			-32.240	20.988	82.669	1.00	50.72
1405	CA	GLY			-32.155	20.071	81.553		49.63
1406	C	GLY			-33.262	20.211	80.509	1.00	49.30
1407	Ö	GLY			-33.624	19.227	79.864		50.60
1408	N	ARG			-33.809	21.402	80.323	1.00	47.24
1409	CA	ARG			-34.799	21.609	79.256	1.00	46.04
1410	CB	ARG			-35.716	22.800	79.591	1.00	46.73
1411	CG	ARG			-36.712	22.504	80.773	1.00	49.63
1412						23.759		1.00	
	CD	ARG			-37.419		81.406		55.75
1413	NE	ARG			-37.497	24.898	80.477	1.00	58.41
1414	CZ	ARG			-37.277	26.172	80.822	1.00	60.70
1415	NH1	ARG			-37.360	27.151	79.903		61.20
1416	NH2	ARG			-36.965	26.473	82.083	1.00	58.65
1417	С	ARG			-34.097	21.838	77.907		44.67
1418	0	ARG			-32.861	21.996	77.852		43.50
1419	N	MET	Α	305	-34.858	21.822	76.819	1.00	41.82

FIGURE 3AB

A	В	С	D	Ε		F	G	Н	I	J
1420	CA	MET	Α	305		-34.254	22.089	75.503	1.00	42.19
1421	CB	MET	Α	305	-	-35.229	21.851	74.333	1.00	41.21
1422	CG	MET	Α	305	-	35.426	20.357	73.940	1.00	49.17
1423	SD	MET	Α	305	-	-33.904	19.263	73.897	1.00	58.33
1424	CE	MET	Α	305		-33.530	19.109	72.178	1.00	55.74
1425	C	MET	Α	305	-	-33.865	23.563	75.506	1.00	38.86
1426	0	MET		305		-34.562	24.353	76.091	1.00	38.98
1427	N	HIS	Α	306		32.786	23.933	74.838	1.00	37.11
1428	CA			306		-32.358	25.332	74.903	1.00	36.23
1429	CB	HIS		306		-31.486	25.515	76.164	1.00	34.70
1430	CG	HIS		306		-30.350	24.541	76.239	1.00	31.57
1431		HIS				-30.436	23.353	76.920	1.00	30.19
1432	CE1		Α	306		29.306	22.688	76.809	1.00	31.98
1433				306		-28.485	23.405	76.061	1.00	33.02
1434		HIS		306		-29.117	24.569	75.698	1.00	31.19
1435	C	HIS	Α	306		-31.570	25.711	73.662	1.00	36.80
1436	0			306		-31.106	24.834	72.897	1.00	36.60
1437 1438	N CA	ASP		307		-31.378 -30.728	27.017	73.498 72.310	1.00	37.06 37.90
1438	CB	ASP		307		-30.728	27.538 27.990	71.294	1.00	38.38
1440	CG			307		-32.671	29.159	71.294	1.00	43.93
1441		ASP				-33.590	29.626	71.077	1.00	51.28
1442		ASP		307		-32.554	29.695	72.926	1.00	43.92
1443	C	ASP				29.824	28.702	72.622	1.00	37.59
1444	Ö	ASP				-29.361	28.848	73.739	1.00	37.38
1445	N	GLU		308		-29.676	29.585	71.642	1.00	36.80
1446	CA			308		-28.726	30.683	71.742	1.00	37.37
1447	CB	GLU		308		-28.825	31.551	70.492	1.00	37.85
1448	CG	GLU	Α	308	-	-28.228	30.905	69.266	1.00	40.29
1449	CD	GLU	Α	308	-	-29.197	29.990	68.528	1.00	45.91
1450	OE1	GLU	Α	308	-	-30.253	29.629	69.089	1.00	43.52
1451	OE2	GLU	Α	308	-	-28.879	29.616	67.361	1.00	48.59
1452	C	GLU		308		-29.008	31.574	72.946	1.00	35.64
1453	0			308		-28.099	32.237	73.434	1.00	34.56
1454	N	LYS		309		-30.247	31.603	73.410	1.00	33.77
1455	CA	LYS		309		-30.557	32.491	74.535	1.00	33.68
1456	CB			309		-32.071	32.589	74.813	1.00	34.13
1457	CG	LYS	Α	309		-32.853	33.190	73.626	1.00	35.58
1458	CD			309		-32.289	34.571	73.302	1.00	39.16
1459 1460	CE			309		-33.289 -34.624	35.387	72.485 73.121	1.00	46.27
1460	NZ C	LYS		309 309		-34.624	35.259 32.123	75.816	1.00	46.60 32.90
1462	0			309		-29.793	32.123	76.708	1.00	32.40
1462	N			310		-29.073	30.932	75.870	1.00	31.17
1464	CA	VAL		310		-28.473	30.508	77.022	1.00	32.76
1465	CB	VAL		310		27.993	29.086	76.822	1.00	33.19
1466	CG1	VAL		310		26.762	28.825	77.639	1.00	36.49
1467	CG2	VAL		310		-29.154	28.095	77.249	1.00	32.68
1468	C	VAL		310		-27.292	31.457	77.250	1.00	33.09
1469	ō	VAL				-27.083	31.951	78.365	1.00	31.77
1470	N	ASP	Α	311		26.568	31.770	76.175		31.32

FIGURE 3AC

A I	В	С	D	E	F	G	H	1	J
1471 (CA	ASP	Α	311	-25.422	32.682	76.275	1.00	32.19
		ASP			-24.578	32.656	74.950	1.00	32.21
	CG	ASP			-23.893	31.256	74.696	1.00	33.63
		ASP			-23.601	30.482	75.635		34.07
		ASP			-23.615	30.806	73.584		34.64
	502	ASP			-25.848	34.089	76.674		31.34
	5	ASP			-25.054	34.819	77.265	1.00	31.50
	y V	LEU			-27.074	34.500	76.349	1.00	30.65
	CA.	LEU			-27.540	35.829	76.741		30.65
	CB	LEU			-28.880 -28.740	36.194 36.747	76.114 74.676	1.00	32.89
	CG	LEU						1.00	33.15
		LEU			-27.998	38.080	74.782	1.00	37.24
		LEU			-27.978	35.740	73.770	1.00	37.98
	2	LEU			-27.659	35.915	78.252		30.10
	0	LEU			-27.212	36.882	78.870		29.74
	N	TRP			-28.221	34.878	78.847		28.70
	CA	TRP			-28.290	34.885	80.311		29.18
	CB	TRP			-28.980	33.655	80.774	1.00	29.28
	CG	TRP			-28.856	33.398	82.197		29.13
	CD1	TRP			-27.798	32.871	82.848		26.72
	NE1	TRP			-28.104	32.728	84.184		28.25
		TRP			-29.402	33.129	84.370		28.86
	CD2	TRP			-29.877	33.584	83.145	1.00	26.93
1494 (CE3	TRP	Α	313	-31.192	34.028	83.062	1.00	26.93
1495 (CZ3	TRP			-31.969	34.038	84.199	1.00	31.77
1496 (CH2	TRP	Α	313	-31.450	33.635	85.422	1.00	28.09
1497 (CZ2	TRP	Α	313	-30.175	33.170	85.538	1.00	26.06
1498 (2	TRP	Α	313	-26.880	34.959	80.918	1.00	29.84
1499 (С	TRP	Α	313	-26.633	35.738	81.823	1.00	27.08
1500 1	N	SER	Α	314	-25.958	34.152	80.409	1.00	29.72
1501 (CA	SER	Α	314	-24.593	34.162	80.901	1.00	30.37
1502 (CB	SER	Α	314	-23.777	33.087	80.139	1.00	30.46
1503 (OG	SER	Α	314	-24.244	31.776	80.494	1.00	35.30
1504 (3	SER	Α	314	-23.937	35.568	80.801	1.00	31.13
1505 (С	SER	Α	314	-23.199	35.980	81.679	1.00	27.77
1506 1	N	LEU	Α	315	-24.183	36.276	79.708	1.00	30.52
1507	CA	LEU	Α	315	-23.699	37.630	79.537	1.00	31.47
1508	CB	LEU	Α	315	-24.303	38.182	78.258	1.00	31.92
1509 (CG	LEU	Α	315	-23.556	39.322	77.630	1.00	34.89
1510 (CD1	LEU	Α	315	-22.077	38.966	77.617	1.00	32.65
1511 (CD2	LEU	Α	315	-24.094	39.490	76.207	1.00	34.24
1512 (2	LEU	Α	315	-24.189	38.521	80.657	1.00	30.26
1513 (0	LEU	Α	315	-23.467	39.375	81.154	1.00	29.93
1514 1	N	GLY	Α	316	-25.416	38.270	81.084	1.00	31.24
1515 (CA	GLY	Α	316	-26.030	39.018	82.160	1.00	28.40
		GLY			-25.336	38.709	83.470		29.31
		GLY			-24.989	39.635	84.232	1.00	28.62
		VAL			-25.123	37.426	83.751	1.00	29.39
		VAL			-24.392	37.045	84.964		29.86
		VAL			-24.272	35.498	85.118		29.69
		VAL			-23.433	35.135	86.302		31.40
'									

FIGURE 3AD

Α	В	С	D	Е	F	G	H	1	J
1522	CG2	VAL	Α	317	-25.625	34.885	85.201	1.00	30.52
1523	C	VAL	Α	317	-22.971	37.715	84.961	1.00	30.09
1524	0	VAL	Α	317	-22.525	38.275	85.976	1.00	28.93
1525	N	LEU	Α	318	-22.283	37.665	83.832	1.00	29.07
1526	CA	LEU	Α	318	-20.973	38.219	83.759	1.00	29.74
1527	CB	LEU	Α	318	-20.327	37.940	82.391	1.00	29.62
1528	CG	LEU	Α	318	-19.795	36.566	82.116	1.00	33.45
1529	CD1	LEU	Α	318	-19.343	36.587	80.606	1.00	31.59
1530	CD2	LEU	Α	318	-18.570	36.186	83.001	1.00	26.99
1531	C			318	-21.015	39.716	83.938	1.00	29.78
1532	0	LEU			-20.140	40.243	84.572	1.00	29.27
1533	N			319	-22.036	40.401	83.423	1.00	29.91
1534	CA			319	-22.072	41.831	83.606	1.00	31.51
1535	CB	CYS		319	-23.214	42.431	82.818	1.00	31.68
1536	SG			319	-23.007	44.241	82.719	1.00	40.49
1537	С			319	-22.152	42.216	85.116	1.00	31.22
1538	0	CYS			-21.439	43.092	85.632	1.00	29.46
1539	N	TYR			-22.985	41.482	85.819	1.00	29.74
1540	CA			320	-23.149	41.689	87.243	1.00	28.88
1541	CB			320	-24.320	40.843	87.746	1.00	28.54
1542	CG			320	-24.606	40.973	89.212	1.00	28.67
1543	CD1	TYR			-23.746	40.436	90.152	1.00	28.63
1544	CE1	TYR			-24.037	40.574	91.521	1.00	31.25
1545 1546	CZ	TYR		320	-25.218 -25.601	41.261	91.901 93.204	1.00	27.73
1547	OH CE2	TYR		320 320	-26.070	41.711	91.016	1.00	28.41
1548	CD2	TYR		320	-25.745	41.625	89.636	1.00	27.53
1549	C			320	-21.810	41.373	87.977	1.00	29.65
1550	0			320	-21.286	42.208	88.741	1.00	28.99
1551	N	GLU			-21.252	40.185	87.727	1.00	28.26
1552	CA	GLU			-19.996	39.790	88.381	1.00	29.29
1553	CB	GLU		321	-19.511	38.398	87.976	1.00	27.46
1554	CG	GLU			-18.367	37.989	88.874	1.00	31.39
1555	CD			321	-17.939	36.565	88.757	1.00	39.04
1556	OE1	GLU		321	-16.893	36.204	89.386	1.00	40.16
1557	OE2	GLU	Α	321	-18.629	35.792	88.062	1.00	41.43
1558	C	GLU	Α	321	-18.858	40.810	88.173	1.00	29.09
1559	0	GLU	Α	321	-18.148	41.162	89.112	1.00	28.70
1560	N	PHE	Α	322	-18.712	41.290	86.942	1.00	28.18
1561	CA	PHE	Α	322	-17.690	42.282	86.620	1.00	29.59
1562	CB	PHE	Α	322	-17.742	42.671	85.130	1.00	30.02
1563	CG	PHE		322	-17.277	41.578	84.189	1.00	29.13
1564	CD1			322	-16.706	40.416	84.659	1.00	29.70
1565	CE1	PHE		322	-16.287	39.422	83.772	1.00	32.17
1566	CZ	PHE		322	-16.416	39.619	82.418	1.00	33.54
1567	CE2	PHE		322	-16.981	40.753	81.954	1.00	33.04
1568	CD2	PHE	Α	322	-17.412	41.738	82.844	1.00	30.45
1569	С	PHE			-17.874	43.526	87.468	1.00	30.51
1570	0			322	-16.924	44.017	88.092	1.00	32.18
1571	N	LEU			-19.079	44.047	87.443	1.00	30.76
1572	CA	LEU	Α	323	-19.461	45.235	88.188	1.00	31.93

FIGURE 3AE

A	В	С	D	E		F	G	H	1	J
1573	CB	LEU	Α	323	-20.	.850	45.703	87.765	1.00	31.23
1574	CG	LEU	Α	323	-21.	.005	46.300	86.372	1.00	29.55
1575	CD1	LEU	Α	323	-22.	.381	46.696	86.162	1.00	28.14
1576		LEU			-20		47.538	86.199		33.58
1577	c	LEU			-19		45.015	89.689		33.43
1578	ō	LEU			-19		45.912	90.469		33.54
1579	N	VAL			-19		43.827	90.139		33.63
1580	CA	VAL			-20		43.630	91.587	1.00	33.28
1581	CB	VAL			-21.		42.976	91.860		33.80
1582	CG1	VAL			-21.		42.622	93.380		32.67
1583	CG2	VAL			-22.		43.857	91.300		34.21
1584	C	VAL			-18		42.911	92.263		35.51
1585	Ö	VAL			-18		43.145	93.424		35.39
1586	N	GLY			-18		42.038	91.560		35.56
1587	CA	GLY			-17.		41.273	92.225		35.35
1588	C	GLY			-17		39.835	92.535		36.00
1589	Ö	GLY			-16		39.003	92.813		37.09
1590	N			326	-18		39.528	92.442	1.00	35.21
1591	CA			326	-19.		38.161	92.638		35.82
1592	CB			326	-19.		37.922	94.122		35.98
1593	CG			326	-20.		38.598	94.489	1.00	40.08
1594	CD			326	-21.		38.587	96.024		47.40
1595	CE	LYS			-22		39.748	96.321		51.86
1596	NZ			326	-21		40.553	97.484		48.80
1597	C			326	-20		37.929	91.754		33.85
1598	0	LYS			-21		38.853	91.451	1.00	31.55
1599	N			327	-20.		36.691	91.332	1.00	33.50
1600	CA			327	-21.		36.437	90.463	1.00	32.79
1601	CB	PRO			-21.		34.994	89.969		33.94
1602	CG	PRO			-21.		34.347	91.241		35.31
1603	CD	PRO			-19.		35.449	91.621		33.33
1604	C	PRO			-23.		36.595	91.255		30.81
1605	Ö	PRO			-23.		36.380	92.463	1.00	32.11
1606	N	PRO			-24		36.989	90.598		29.67
1607	CA			328	-25		37.336	91.315		29.91
1608	CB			328	-26		37.936	90.249		28.24
1609	CG	PRO			-25		37.253	88.972	1.00	30.64
1610	CD			328	-24		37.239	89.158	1.00	29.03
1611	C	PRO			-26		36.189	92.066		32.07
1612	ō	PRO			-27		36.498	92.935		31.51
1613	N	PHE			-26.		34.919	91.745	1.00	30.77
1614	CA	PHE			-26.		33.835	92.391	1.00	32.15
1615	CB			329	-27		32.923	91.329	1.00	30.34
1616	CG			329	-28		33.663	90.371		29.16
1617	CD1	PHE			-29		34.294	90.783	1.00	26.86
1618	CE1	PHE			-30		35.003	89.921	1.00	26.79
1619	CZ			329	-29.		35.115	88.583		29.19
1620	CE2	PHE			-28.		34.503	88.156	1.00	28.24
1621	CD2	PHE			-27		33.782	89.042		29.12
1622	С	PHE			-25.		33.027	93.287		33.34
1623	0	PHE			-26.		31.988	93.763		35.58

FIGURE 3AF

A	В	С	D	Е		F		G	1	Н		Ι	J
1624	N	GLU	Α	330	-2	4.623	33.	.505	93	.513	1	.00	35.42
1625	CA	GLU	Α	330	-23	3.656	32.	.877	94	.397	1	.00	38.76
1626	CB	GLU				2.588		906		.768		.00	39.72
1627	CG	GLU				1.251		.325	95	.177		.00	44.21
1628	CD	GLU				0.378		.364		.894		.00	53.19
1629	OE1			330		0.779		.883		.993		.00	53.55
1630	OE2	GLU				9.295		.665		.337		.00	58.16
1631	C	GLU				4.373		.498		.704		.00	39.04
1632	0	GLU				5.175		.269		.217		.00	37.84
1633	N	ALA	Α	331		4.084	31.	.303	96	.200	1	.00	40.28
1634	CA	ALA				4.680		.771		.425		.00	40.27
1635	CB	ALA				6.002		.149		.126		.00	41.00
1636	C	ALA				3.658		.753		.888		.00	41.45
1637	0	ALA				2.757		.404		.127		.00	41.16
1638	N	ASN			-23	3.776	29.	.280	99	.121		.00	41.89
1639	CA	ASN	Α	332	-22	2.737	28.	.404	99	.662	1	.00	40.88
1640	CB	ASN				2.602		.566		.220		.00	43.11
1641	CG	ASN				1.784		.826		.626		.00	48.66
1642	OD1	ASN				0.570		.937		.359		.00	55.22
1643	ND2	ASN				2.462		.786		.245		.00	55.15
1644	C	ASN			-2:	3.050	26.	959	99	.235		.00	37.57
1645	0	ASN				2.225		.050		.332		.00	39.59
1646	N	THR				4.231		.755		.724		.00	36.44
1647	CA	THR				4.536		.410		.298		.00	36.73
1648	CB	THR				5.645		.665		.264		.00	37.09
1649	OG1	THR		333		5.097		.779		.596		.00	40.58
1650	CG2	THR	Α	333		5.650	23.	.188		.046	1	.00	42.78
1651	С	THR	Α	333	-24	4.981	25.	.425	96	.865		.00	34.33
1652	0	THR				5.642		.372		.398		.00	33.08
1653	N	TYR			-2	4.713	24.	.319		.190	1	.00	34.09
1654	CA	TYR				5.181		.137		.830		.00	33.28
1655	CB	TYR			-2	4.748	22.	.746	94	.425	1	.00	34.15
1656	CG	TYR	Α	334	-25	5.241	22.	.198	93	.148	1	.00	35.67
1657	CD1	TYR	Α	334	-2	4.367	22.	.102	92	.069	1	.00	39.34
1658	CE1	TYR	Α	334	-24	4.765	21.	.536		.885	1	.00	41.47
1659	CZ	TYR	Α	334	-26	6.025	21.	.028	90	.764	1	.00	45.44
1660	OH	TYR	Α	334	-26	6.316	20.	.439	89	.536	1	.00	53.44
1661	CE2	TYR	Α	334	-26	6.931	21.	.076	91	.822	1	.00	41.49
1662	CD2	TYR	Α	334	-26	6.535	21.	.644	93	.021	1	.00	39.26
1663	С	TYR	Α	334	-26	6.682	24.	.162	94	.837	1	.00	34.00
1664	0	TYR	Α	334	-2	7.330	24.	.686	93	.921	1	.00	32.29
1665	N	GLN	Α	335	-21	7.263	23.	.490	95	.830	1	.00	33.92
1666	CA	GLN	Α	335	-28	8.698	23.	.382	95	.856	1	.00	34.59
1667	CB	GLN	Α	335	-29	9.136	22.	.355	96	.934	1	.00	36.44
1668	CG	GLN	Α	335	-21	8.819	20.	855	96	.503	1	.00	37.94
1669	CD	GLN	Α	335	-2	7.495	20.	.276	97	.085	1	.00	40.55
1670	OE1	GLN	Α	335	-2"	7.461	19.	.102	97	.552	1	.00	37.86
1671	NE2	GLN		335		6.437		.088		.108		.00	36.60
1672	C	GLN	Α	335		9.324	24.	.794	96	.037	1	.00	34.20
1673	0	GLN				0.282		.140		.379		.00	35.30
1674	N	GLU	Α	336		8.791		.559		.942		.00	32.77

FIGURE 3AG

A	В	С	D	E	F	G	H	I	J
1675	CA	GLU	А	336	-29.205	26.915	97.201	1.00	34.44
1676	CB	GLU			-28.385	27.265	98.440	1.00	36.83
1677	CG	GLU	Α	336	-28.352	28.650	99.013	1.00	40.38
1678	CD	GLU	Α	336	-27.092	28.866	99.875	1.00	50.58
1679	OE1	GLU	Α	336	-25.978	28.319	99.620	1.00	58.53
1680	OE2	GLU	Α	336	-27.126	29.678	100.790	1.00	40.31
1681	С	GLU	Α	336	-28.995	27.811	95.873	1.00	33.80
1682	0	GLU	Α	336	-29.877	28.563	95.449	1.00	31.17
1683	N	THR	Α	337	-27.868	27.635	95.191	1.00	32.08
1684	CA	THR			-27.662	28.368	93.945	1.00	31.48
1685	CB	THR	Α	337	-26.235	28.047	93.405	1.00	30.08
1686	OG1	THR			-25.313	28.487	94.390	1.00	33.00
1687	CG2				-25.906	28.929	92.159	1.00	28.28
1688	C			337	-28.724	28.055	92.919	1.00	29.52
1689	0			337	-29.235	28.932	92.247	1.00	28.46
1690	N	TYR		338	-29.027	26.756	92.754	1.00	30.17
1691	CA			338	-30.049	26.309	91.844	1.00	31.26
1692	CB			338	-30.212	24.805	92.063	1.00	33.22
1693	CG			338	-31.212	24.185	91.144	1.00	39.22
1694	CD1	TYR			-30.800	23.567	89.964	1.00	43.19
1695	CE1	TYR			-31.709	22.969	89.124	1.00	48.41
1696 1697	CZ			338	-33.058 -33.992	23.003	89.460	1.00	51.06
1698	OH CE2	TYR		338	-33.479	22.431 23.615	88.628 90.622	1.00	46.29
1699	CD2	TYR			-32.560	24.179	91.462	1.00	40.23
1700	C			338	-31.396	27.002	92.147	1.00	30.29
1701	0			338	-32.102	27.472	91.277	1.00	29.01
1702	N	ALA			-31.739	27.026	93.411	1.00	29.94
1703	CA	ALA			-32.984	27.737	93.804	1.00	30.96
1704	CB	ALA			-33.149	27.684	95.338	1.00	30.49
1705	C	ALA			-32.960	29.196	93.377	1.00	29.24
1706	0	ALA			-33.915	29.676	92.798	1.00	30.50
1707	N	ARG	Α	340	-31.867	29.875	93.686	1.00	28.80
1708	CA	ARG	Α	340	-31.708	31.285	93.348	1.00	29.69
1709	CB	ARG	Α	340	-30.375	31.804	93.896	1.00	29.56
1710	CG	ARG	Α	340	-30.447	31.776	95.494	1.00	34.62
1711	CD	ARG		340	-31.154	32.954	96.011	1.00	39.53
1712	NE	ARG			-30.493	34.042	95.311	1.00	45.06
1713	CZ	ARG		340	-29.323	34.499	95.716	1.00	45.59
1714	NH1				-28.683	35.456	95.038	1.00	44.01
1715		ARG			-28.835	33.995	96.846	1.00	44.77
1716	C	ARG			-31.871	31.547	91.858	1.00	29.56
1717	0	ARG			-32.649	32.431	91.413	1.00	29.84
1718	N	ILE		341	-31.248	30.679	91.087	1.00	29.70
1719	CA CB			341	-31.279	30.831	89.641	1.00	27.75
1720 1721	CB CG1	ILE		341	-30.265 -28.835	29.851	89.077 89.281	1.00	24.64
1721	CD1	ILE		341	-28.835	29.268	88.849	1.00	27.34
1723	CG2	ILE		341	-30.531	29.617	87.612	1.00	28.09
1724	C			341	-32.653	30.582	89.129	1.00	
1725	0			341	-33.236	31.391	88.388		29.33
	-	- 222							

FIGURE 3AH

A	В	C	D	Ε		F		G	1	H	1	J
1726	N	SER	Α	342	-3	3.258	29	.478	89	.585	1.00	30.95
1727	CA	SER	Α	342	-3	4.581	29	.093	89	.125	1.00	31.90
1728	CB	SER	Α	342	-3	4.973	27	.779	89	.822	1.00	33.11
1729	OG			342		6.337		.538	89	.665	1.00	42.55
1730	C			342		5.593		.214		400		32.49
1731	Ö			342		6.445		.492		.565	1.00	35.12
1732	N	ARG		343		5.471		.872		.559	1.00	31.84
1733	CA	ARG				6.386		.949		.917	1.00	32.56
1734	CB	ARG				6.532		.017		470		33.12
1735	CG	ARG				7.178		.751		.099	1.00	36.80
1736	CD	ARG				6.953		.623		.628	1.00	43.39
1737	NE	ARG				7.670		.540		.344	1.00	52.05
1738	CZ	ARG				8.085		.360		.847	1.00	55.23
1739	NH1	ARG				7.862		.015		.587		58.10
1740	NH2	ARG				8.717		.495		.654	1.00	
1741	C	ARG				5.914		.324		.386	1.00	32.02
1742	0	ARG		343		6.648		.286		.481	1.00	31.13
1743	N	VAL				4.717		.360		.766	1.00	32.93
1744	CA	VAL				4.045		.613		.312		33.02
1745	CB	VAL				4.600		.259		.032		33.79
1746	CG1	VAL				3.546		.165		.403	1.00	33.57
1747	CG2	VAL				5.020		.205		.041	1.00	34.92
1748	C	VAL				3.993		.587		.479	1.00	31.91
1749	Ö	VAL				4.392		.741		.393		32.52
1750	N	GLU				3.500		.117		.597		33.06
1751	CA	GLU				3.507		.977		.743	1.00	35.54
1752	CB	GLU		345		4.047		.248		.988	1.00	37.02
1753	CG	GLU				3.651		.818		.122	1.00	44.67
1754	CD	GLU				4.183		.209		.428	1.00	
1755	OE1	GLU				4.610		.982		.347	1.00	58.06
1756	OE2	GLU				4.139		.965		.554	1.00	58.84
1757	C	GLU				2.132		.606		.961	1.00	33.87
1758	Ö	GLU				1.186		.950		.332	1.00	33.72
1759	N	PHE				2.045		.894		.694		32.77
1760	CA			346		0.811		.628		.902		32.91
1761	CB			346		9.903		.502		.657	1.00	33.13
1762	CG	PHE	A	346		0.431		.197		469	1.00	34.17
1763	CD1			346		1.338		.570		.647	1.00	36.56
1764	CE1			346		1.838		.183		.527		35.71
1765	CZ			346		1.465		.474		.220	1.00	38.88
1766	CE2	PHE				0.569		.142		.037	1.00	38.32
1767		PHE				0.018		.488		.146	1.00	39.09
1768	C	PHE				1.134		.106		.174	1.00	33.06
1769	Ö	PHE				2.209		.598		.785		32.92
1770	N	THR				0.225		.796		.853	1.00	32.73
1771	CA	THR				0.385		.225		.108	1.00	33.76
1772	CB	THR		347		0.753		.502		.597	1.00	33.91
1773	OG1	THR				9.776		.870		.415	1.00	35.21
1774	CG2	THR				2.067		.798		.015	1.00	33.87
1775	CGZ	THR				9.025		.839		.850		33.74
1776	0	THR				7.998		.142		.915		34.60
1110	J	1111	n	24/	-2		42	. 142	23	. 213	1.00	J4.00

FIGURE 3AI

A	В	C	D	Е	F	G	H	1	J
1777	N	PHE	Α	348	-29.028	44.146	93.635	1.00	33.51
1778	CA	PHE	Α	348	-27.835	44.911	93.268	1.00	33.28
1779	CB			348	-28.204	45.979	92.254	1.00	32.67
1780	CG	PHE	Α	348	-28.626	45.454	90.940	1.00	31.24
1781	CD1	PHE	Α	348	-29.962	45.538	90.551	1.00	32.35
1782	CE1	PHE	Α	348	-30.374	45.068	89.325	1.00	31.74
1783	CZ	PHE		348	-29.433	44.491	88.447	1.00	30.42
1784	CE2	PHE	Α	348	-28.090	44.411	88.822	1.00	32.15
1785	CD2	PHE			-27.695	44.892	90.070	1.00	30.97
1786	C	PHE	Α	348	-27.337	45.701	94.453	1.00	35.77
1787	0	PHE	Α	348	-28.126	46.255	95.209	1.00	35.76
1788	N	PRO	Α	349	-26.025	45.772	94.628	1.00	36.99
1789	CA	PRO	Α	349	-25.493	46.699	95.626	1.00	37.46
1790	CB	PRO	Α	349	-23.963	46.485	95.567	1.00	38.56
1791	CG	PRO	Α	349	-23.670	45.526	94.471	1.00	37.30
1792	CD	PRO	Α	349	-24.990	45.029	93.906	1.00	37.24
1793	C	PRO	Α	349	-25.883	48.098	95.159	1.00	37.57
1794	0	PRO	Α	349	-26.153	48.337	93.990	1.00	36.04
1795	N	ASP	Α	350	-25.921	49.055	96.076	1.00	39.36
1796	CA	ASP	Α	350	-26.257	50.422	95.693	1.00	40.98
1797	CB	ASP	Α	350	-26.206	51.348	96.903	1.00	42.59
1798	CG	ASP	Α	350	-27.260	51.031	97.914	1.00	47.11
1799	OD1	ASP	Α	350	-27.128	51.620	99.016	1.00	53.92
1800	OD2	ASP	Α	350	-28.222	50.225	97.689	1.00	50.42
1801	C	ASP	Α	350	-25.351	51.058	94.663	1.00	40.13
1802	0	ASP	Α	350	-25.814	51.905	93.909	1.00	40.28
1803	N	PHE	Α	351	-24.063	50.736	94.649	1.00	39.85
1804	CA	PHE	Α	351	-23.202	51.402	93.673	1.00	39.47
1805	CB	PHE	Α	351	-21.718	51.213	93.957	1.00	40.21
1806	CG	PHE			-21.278	49.784	93.967		41.11
1807	CD1	PHE			-21.221	49.082	95.162		39.89
1808	CE1	PHE			-20.833	47.761	95.192	1.00	40.56
1809	CZ	PHE			-20.521	47.111	93.978		42.46
1810	CE2				-20.589	47.826	92.772	1.00	39.35
1811	CD2				-20.977	49.124	92.767		41.22
1812	С	PHE			-23.543	51.116	92.213	1.00	40.90
1813	0	PHE			-23.177	51.889	91.325	1.00	41.02
1814	N	VAL			-24.278	50.042	91.927	1.00	39.58
1815	CA	VAL			-24.604	49.759	90.531	1.00	38.85
1816	CB	VAL			-25.223	48.351	90.345	1.00	37.90
1817		VAL			-25.491	48.084	88.893	1.00	36.19
1818		VAL			-24.271	47.308	90.902	1.00	38.04
1819	С	VAL			-25.531	50.764	89.905	1.00	39.39
1820	0	VAL			-26.631	50.985	90.420	1.00	38.87
1821	N	THR			-25.136	51.309	88.742		40.16
1822	CA	THR			-25.943	52.332	88.057	1.00	40.56
1823	CB	THR			-25.127	53.080	86.987	1.00	41.20
1824	OG1	THR			-24.703	52.160	85.970	1.00	39.47
1825	CG2	THR			-23.893	53.625	87.588	1.00	39.13
1826 1827	C	THR			-27.216 -27.424	51.852 50.664	87.400 87.152		41.64
102/	0	THK	14	333	-21.424	30.004	0/.152	1.00	41.19

FIGURE 3AJ

A	В	С	D	E	F	G	Н	1	J
1828	N	GLU	Α	354	-28.071	52.816	87.102	1.00	41.67
1829	CA	GLU	Α	354	-29.321	52.514	86.485	1.00	43.44
1830	CB	GLU	Α	354	-30.191	53.770	86.372	1.00	46.05
1831	CG	GLU			-30.592	54.252	87.751		54.41
1832	CD	GLU			-30.894	53.090	88.684		64.52
1833	OE1	GLU			-32.014	52.505	88.550	1.00	68.68
1834	OE2	GLU			-30.038	52.775	89.551	1.00	
1835	C	GLU			-29.168	51.828	85.156	1.00	41.54
1836	o	GLU			-29.908	50.900	84.858	1.00	40.38
1837	N	GLY			-28.226	52.291	84.353	1.00	
1838	CA	GLY			-28.041	51.714	83.044	1.00	37.79
1839	C	GLY			-27.598	50.271	83.170	1.00	36.84
1840	Ö	GLY			-28.060	49.403	82.423	1.00	37.14
1841	N	ALA			-26.684	50.016	84.092		36.29
1842	CA	ALA			-26.178	48.669	84.268		36.41
1843	CB	ALA			-24.998	48.660	85.206	1.00	35.64
1844	C	ALA			-27.295	47.794	84.782	1.00	35.70
1845	Ö	ALA			-27.490	46.695	84.309	1.00	34.90
1846	N	ARG			-28.072	48.293	85.745		36.25
1847	CA	ARG			-29.186	47.504	86.264		36.61
1848	CB	ARG			-29.960	48.250	87.339	1.00	36.86
1849	CG	ARG			-29.169	48.482	88.582	1.00	34.77
1850	CD	ARG			-29.988	49.289	89.609	1.00	37.61
1851	NE	ARG			-29.112	49.640	90.708		36.40
1852	CZ	ARG			-29.400	49.468	91.975		35.35
1853	NH1	ARG			-30.572	48.952	92.320	1.00	39.15
1854	NH2	ARG			-28.498	49.787	92.890	1.00	33.56
1855	C	ARG			-30.165	47.167	85.172	1.00	37.12
1856	o	ARG			-30.718	46.074	85.153		37.21
1857	N	ASP			-30.420	48.132	84.297		37.24
1858	CA	ASP			-31.353	47.925	83.226	1.00	37.93
1859	CB	ASP			-31.614	49.202	82.454	1.00	38.87
1860	CG	ASP			-32.621	48.984	81.324	1.00	
1861		ASP			-33.846	49.000	81.602		46.16
1862	OD2	ASP			-32.290	48.788	80.126	1.00	45.46
1863	C	ASP			-30.868	46.836	82.281	1.00	36.98
1864	ō	ASP			-31.656	45.967	81.884	1.00	36.97
1865	N	LEU			-29.578	46.860	81.942	1.00	35.72
1866	CA	LEU			-29.042	45.867	81.031		35.51
1867	CB	LEU			-27.595	46.168	80.713		35.38
1868	CG	LEU			-27.063	45.779	79.327	1.00	39.30
1869	CD1				-25.507	45.577	79.301	1.00	37.82
1870	CD2	LEU			-27.787	44.681	78.634	1.00	35.07
1871	Ċ	LEU			-29.127	44.477	81.657	1.00	33.71
1872	0	LEU			-29.575	43.515	81.028		32.97
1873	N			360	-28.679	44.388	82,900	1.00	32.44
1874	CA			360	-28.646	43.105	83.610	1.00	31.57
1875	CB			360	-27.847	43.253	84.926	1.00	31.85
1876	CG1	ILE			-26.367	43.490	84.572	1.00	32.47
1877	CD1			360	-25.639	44.299	85.549		29.24
1878	CG2				-27.934	41.956	85.801		30.72

FIGURE 3AK

A	В	C	D	Е		F	G	H	1	J
1879	С	ILE	Α	360	-30.	053	42.521	83.830	1.00	32.40
1880	0	ILE	Α	360	-30.	265	41.308	83.611	1.00	31.17
1881	N	SER	Α	361	-30.	996	43.386	84.214	1.00	32.23
1882	CA			361	-32.		42.958	84.445	1.00	34.85
1883	CB			361	-33.		44.060	85.087		35.23
1884	OG			361	-32.		44.245	86.443	1.00	40.29
1885	C			361	-32.		42.457	83.143	1.00	34.58
1886	o			361	-33.		41.528	83.147	1.00	34.46
1887	N			362	-32.		43.020	82.017		35.27
1888	CA	ARG			-33.		42.553	80.736		35.84
1889	CB	ARG			-32.		43.595	79.653	1.00	36.24
1890	CG	ARG			-33.		44.805	79.768		42.24
1891	CD	ARG			-33.		46.000	78.930		48.93
1892	NE	ARG			-34.		47,177	79.139		57.80
1893	CZ			362	-34.		47.717	78.208		63.64
1894	NH1	ARG			-34.		47.208	76.972	1.00	67.52
1895	NH2	ARG			-35.		48.771	78.502		65.50
1896	C			362	-32.		41.220	80.283	1.00	35.03
1897	Ö			362	-33.		40.429	79.634		36.42
1898	N			363	-31.		40.939	80.664		32.41
1899	CA			363	-30.		39.705	80.279	1.00	32.03
1900	CB			363	-29.		39.896	80.329	1.00	31.58
1901	CG			363	-28.		40.365	79.163	1.00	34.89
1902	CD1	LEU			-28.		40.467	77.803		36.09
1903	CD2	LEU			-27.		41.450	79.528		34.69
1904	C			363	-31.		38.572	81.203	1.00	32.15
1905	Ö			363	-31.		37.430	80.776	1.00	33.41
1906	N			364	-31.		38.857	82.472	1.00	31.16
1907	CA			364	-31.		37.770	83.428		32.01
1908	CB			364	-30.		38.067	84.804		31.60
1909	CG			364	-29.		38.146	84.738	1.00	31.16
1910	CD1				-28.		38.468	86.102	1.00	34.77
1911	CD2	LEU	Α	364	-28.	841	36.783	84.213	1.00	31.53
1912	C	LEU	Α	364	-33.	088	37.535	83.500	1.00	33.63
1913	0			364	-33.	734	37.811	84.487	1.00	33.26
1914	N	LYS	Α	365	-33.	662	37.065	82.410	1.00	33.41
1915	CA	LYS	Α	365	-35.	082	36.796	82.393	1.00	35.64
1916	CB	LYS	Α	365	-35.	718	37.369	81.135	1.00	35.84
1917	CG	LYS	Α	365	-35.	929	38.880	81.125	1.00	39.34
1918	CD	LYS	Α	365	-36.	633	39.297	82.400	1.00	46.53
1919	CE	LYS	Α	365	-37.	698	40.335	82.107	1.00	49.18
1920	NZ	LYS	Α	365	-37.	064	41.556	81.577	1.00	54.14
1921	C	LYS	Α	365	-35.	216	35.299	82.375	1.00	35.57
1922	0	LYS	Α	365	-34.	516	34.626	81.599	1.00	34.77
1923	N			366	-36.		34.780	83.241		34.63
1924	CA			366	-36.		33.372	83.302	1.00	36.28
1925	CB			366	-37.		33.047	84.346	1.00	35.81
1926	CG			366	-37.		31.581	84.590	1.00	39.29
1927		HIS			-38.		30.728	83.693		41.29
1928	CE1	HIS			-38.		29.487	84.145		40.54
1929	NE2	HIS	Α	366	-37.	446	29.500	85.291	1.00	42.19

FIGURE 3AL

1930 CD2 HIS A 366 -37.088 30.796 85.587 1.00 39.35 1931 C HIS A 366 -36.799 32.856 81.911 1.00 37.30 1932 O HIS A 366 -36.356 31.798 81.435 1.00 36.70 1933 N ASN A 367 -38.095 33.573 81.261 1.00 38.00 1933 C ASN A 367 -38.095 33.598 79.937 1.00 40.15 1935 CB ASN A 367 -40.080 33.074 78.380 1.00 40.85 1936 CG ASN A 367 -40.080 33.074 78.380 1.00 40.28 1937 OD ASN A 367 -40.080 33.074 78.380 1.00 40.28 1938 ND ASN A 367 -40.080 33.074 77.525 1.00 46.36 1938 ND ASN A 367 -39.271 32.476 77.525 1.00 46.36 1938 ND ASN A 367 -37.086 33.524 78.875 1.00 39.35 1940 O ASN A 367 -36.639 33.524 78.875 1.00 39.45 1941 N PRO A 368 -36.397 32.591 78.210 1.00 39.45 1942 CA PRO A 368 -35.363 33.593 77.238 1.00 40.08 1943 CB PRO A 368 -34.976 31.536 76.624 1.00 39.45 1944 CG PRO A 368 -35.451 30.502 77.567 1.00 40.15 1945 CD PRO A 368 -35.451 30.502 77.567 1.00 40.15 1945 CD PRO A 368 -35.624 33.807 76.112 1.00 39.49 1947 O PRO A 368 -35.824 33.807 76.112 1.00 40.68 1948 N SER A 369 -37.064 33.592 75.664 1.00 42.38 1949 CA SER A 369 -37.693 34.457 74.597 1.00 43.95 1950 CB SER A 369 -37.693 34.457 74.597 1.00 43.95 1950 CB SER A 369 -37.693 34.457 74.597 1.00 43.95 1955 CB SER A 369 -37.693 34.457 74.597 1.00 43.95 1955 CB SER A 369 -37.693 34.457 74.597 1.00 43.95 1955 CB SER A 369 -37.692 36.866 75.295 1.00 44.21 1955 CB SER A 369 -37.889 36.754 74.140 1.00 45.51 1955 CB SER A 369 -37.889 36.754 74.140 1.00 45.51 1956 CB SER A 369 -37.889 36.754 74.140 1.00 45.51 1956 CB SER A 369 -37.692 36.866 75.295 1.00 44.21 1955 CB SER A 369 -37.692 36.866 75.295	Α	В	С	D	E		F	G		H	1	J
1932	1930	CD2	HIS	Α	366	-37.	.088	30.79	6 8	5.587	1.00	39.35
1933	1931	С	HIS	Α	366	-36.	.789	32.85	6 8	1.911	1.00	37.30
1934 CA ASN A 367 -38,095 33,069 79,937 1.00 40.10 1935 CB ASN A 367 -40,080 33,074 78,380 1.00 40,428 1937 ODI ASN A 367 -40,080 33,074 78,380 1.00 40,428 1938 ND2 ASN A 367 -39,271 32,476 77,525 1.00 39,35 1939 C ASN A 367 -36,661 34,709 78,683 1.00 34,85 1940 O ASN A 367 -36,661 34,709 78,683 1.00 34,99 1941 N PRO A 368 -36,397 32,591 78,210 1.00 39,49 1942 CA PRO A 368 -35,336 32,903 77,238 1.00 40,08 1943 CB PRO A 368 -35,361 30,590 77,238 1.00 40,08 1944 CG PRO A 368 -34,976 31,536 76,624 1.00 39,29 1945 CD PRO A 368 -35,481 30,502 77,567 1.00 40,15 1945 CD PRO A 368 -35,681 30,502 77,567 1.00 40,15 1946 CC PRO A 368 -35,682 34,684 75,656 1.00 38,95 1948 N SER A 369 -37,692 34,684 75,656 1.00 38,95 1950 CB SER A 369 -37,692 34,437 74,597 1.00 40,48 1951 OS SER A 369 -37,692 34,437 74,597 1.00 40,48 1952 C SER A 369 -37,692 36,186 76,295 1.00 40,40 1955 CB GLN A 370 -37,692 36,186 76,295 1.00 40,40 1955 CB GLN A 370 -37,692 36,186 76,295 1.00 41,21 1959 CB GLN A 370 -37,692 37,264 79,300 1.00 56,48 1960 NEZ GLN A 370 -38,437 37,399 78,053 1.00 44,24 1960 NEZ GLN A 370 -36,213 39,423 77,063 1.00 44,24 1960 NEZ GLN A 370 -36,213 39,423 77,063 1.00 44,24 1960 NEZ GLN A 370 -36,213 39,423 77,063 1.00 44,24 1960 NEZ GLN A 370 -36,213 39,423 77,063 1.00 43,55 1960 CB GRA A 371 -32,118 38,032 78,477 1.00 33,96 1960 CB ARG A 371 -32,118 38,032 78,477 1.00 33,96 1970 NH ARG A 371 -32,291 38,036 74,477 1.00 33,96 1971 NH ARG A 371 -32,291 38,036 74,477 1.00 33,96 1971 NH ARG A 371 -32,291 38,03	1932	0	HIS	Α	366	-36.	.356	31.79	8 8	1.435	1.00	36.00
1935 CB	1933	N	ASN	Α	367	-37.	.684	33.57	3 8	1.261	1.00	38.00
1936 CG ASN A 367 -40,080 33,074 78,380 1,00 44,28 1938 ND2 ASN A 367 -41,276 33,219 78,172 1,00 51,80 1938 ND2 ASN A 367 -39,271 32,2476 77,525 1,00 46,36 1940 O ASN A 367 -36,961 34,709 78,683 1,00 39,35 1941 N PRO A 368 -36,337 32,591 78,210 1,00 39,49 1942 CA PRO A 368 -35,336 32,993 77,238 1,00 40,08 1943 CB PRO A 368 -34,976 31,536 76,624 1,00 39,29 1944 CG PRO A 368 -34,976 31,536 76,624 1,00 39,29 1945 CD PRO A 368 -35,681 30,502 77,567 1,00 40,15 1945 CD PRO A 368 -35,681 30,502 77,567 1,00 40,15 1946 CD PRO A 368 -35,682 31,136 78,295 1,00 40,09 1947 O PRO A 368 -35,682 34,684 75,656 1,00 38,95 1948 N SER A 369 -37,639 34,437 74,597 1,00 43,99 1950 CB SER A 369 -37,639 34,437 74,597 1,00 43,99 1951 OG SER A 369 -37,639 34,437 74,597 1,00 43,99 1952 CS SER A 369 -37,742 35,894 74,995 1,00 44,04 1953 OS SER A 369 -37,742 35,894 74,195 1,00 44,04 1955 CA GIN A 370 -37,742 37,591 76,721 1,00 45,55 1956 CB GIN A 370 -37,692 36,186 76,295 1,00 44,04 1959 CE GIN A 370 -37,692 36,186 76,295 1,00 44,21 1959 CE GIN A 370 -38,437 37,399 78,053 1,00 45,55 1960 CE GIN A 370 -38,437 37,399 78,053 1,00 45,55 1960 CE GIN A 370 -36,232 39,243 77,631 1,00 43,05 1960 CE GIN A 370 -36,232 39,423 77,631 1,00 43,05 1960 CE GIN A 370 -36,232 39,423 77,631 1,00 43,05 1960 CE GIN A 370 -36,232 39,234 77,633 1,00 45,55 1960 CE GIN A 370 -36,232 39,423 77,631 1,00 43,05 1960 CE GIN A 370 -36,232 39,423 77,631 1,00 43,05 1960 CE GIN A 370 -36,232 39,423 77,631 1,00 43,05 1960 CE ARG A 371 -32,118 38,036 7	1934	CA	ASN	Α	367	-38.	.095	33.06	9 7	9.937	1.00	40.10
1938 ND2 ASN A 367 -41.276 33.219 78.172 1.00 51.80 1938 ND2 ASN A 367 -39.271 32.476 77.525 1.00 46.36 1939 C ASN A 367 -36.961 34.709 78.683 1.00 39.35 1940 O ASN A 367 -36.961 34.709 78.683 1.00 39.35 1941 N PRO A 368 -36.397 32.591 78.210 1.00 39.36 1942 CA PRO A 368 -35.336 32.903 77.238 1.00 40.08 1943 CB PRO A 368 -35.336 33.903 77.238 1.00 40.08 1944 CG PRO A 368 -35.345 30.502 77.567 1.00 40.15 1945 CD PRO A 368 -35.451 30.502 77.567 1.00 40.15 1946 C PRO A 368 -35.451 30.502 77.567 1.00 40.15 1947 O PRO A 368 -35.451 30.502 77.567 1.00 40.15 1948 N SER A 369 -37.692 34.684 75.556 1.00 38.95 1949 CA SER A 369 -37.692 34.487 74.597 1.00 43.99 1950 CB SER A 369 -37.693 34.37 74.597 1.00 43.99 1951 OG SER A 369 -37.693 34.37 74.597 1.00 43.99 1952 C SER A 369 -37.692 36.616 73.740 1.00 44.29 1953 OS SER A 369 -37.889 36.754 74.101 1.00 44.29 1954 N GIN A 370 -37.889 36.754 74.995 1.00 44.19 1955 CA GLN A 370 -37.692 36.186 67.295 1.00 44.19 1955 CB GLN A 370 -38.437 37.591 76.721 1.00 45.13 1956 CB GLN A 370 -34.673 37.591 76.921 1.00 50.14 1956 CB GLN A 370 -36.213 38.921 77.694 1.00 50.14 1960 C GLN A 370 -36.213 38.923 77.694 1.00 50.14 1961 C GLN A 370 -36.213 38.923 77.691 1.00 40.95 1962 C GLN A 370 -36.213 38.923 77.692 1.00 36.93 1966 CG GLN A 371 -32.294 36.266 79.474 1.00 63.88 1966 CG ARG A 371 -32.294 36.266 79.474 1.00 33.96 1967 CD ARG A 371 -32.294 36.266 79.474 1.00 33.96 1968 R ARG A 371 -32.291 36.826 79.477 1.00 33.96 1969 CZ ARG A 371 -32.291 36.836 74.377 1.0	1935	CB	ASN	Α	367	-39	.487	33.59	8 7	9.658	1.00	40.85
1938 ND2 ASN A 367 -39.271 32.476 77.525 1.00 46.36 1939 C ASN A 367 -36.6961 34.709 78.683 1.00 39.35 1940 O ASN A 367 -36.6961 34.709 78.683 1.00 39.49 1941 N PRO A 368 -35.336 32.903 77.238 1.00 40.08 1942 CA PRO A 368 -35.336 32.903 77.238 1.00 40.08 1943 CB PRO A 368 -35.481 30.502 77.567 1.00 40.15 1944 CG PRO A 368 -35.481 30.502 77.567 1.00 40.15 1945 CD PRO A 368 -35.681 30.502 77.567 1.00 40.15 1946 C PRO A 368 -35.682 31.136 78.295 1.00 40.09 1947 O PRO A 368 -35.682 34.684 75.656 1.00 38.95 1948 N SER A 369 -37.693 34.437 74.597 1.00 43.99 1950 CB SER A 369 -37.693 34.437 74.597 1.00 43.99 1951 CG SER A 369 -37.693 34.437 74.597 1.00 44.04 1953 O SER A 369 -37.742 35.894 74.995 1.00 44.04 1953 O SER A 369 -37.742 35.894 74.995 1.00 44.04 1955 CA GIN A 370 -37.742 35.864 74.995 1.00 44.04 1955 CA GIN A 370 -37.693 36.186 76.295 1.00 44.04 1955 CA GIN A 370 -37.693 37.264 79.300 1.00 56.48 1960 NE2 GIN A 370 -38.437 37.397 78.053 1.00 45.55 1960 NE2 GIN A 370 -36.233 39.217 79.94 1.00 44.24 1960 NE2 GIN A 370 -36.233 38.256 80.230 1.00 55.95 1960 CG GIN A 370 -36.233 38.256 76.693 1.00 43.05 1960 CG GIN A 370 -36.233 38.257 76.682 1.00 42.30 1960 CG CARG A 371 -32.913 37.927 76.693 1.00 43.05 1960 CG CARG A 371 -32.913 37.927 77.603 1.00 43.05 1970 NH1 ARG A 371 -32.218 37.927 77.506 1.00 33.96 1971 NH2 ARG A 371 -32.218 37.329 77.563 1.00 43.05 1971 NH2 ARG A 371 -32.218 37.940 77.506 1.00 33.96 1972 C ARG A 371 -32.218 37.407 77.507 77.00 37.90 1973 C ARG A 371 -32.218 37.407	1936	CG	ASN	Α	367	-40.	.080	33.07	4 7	8.380	1.00	44.28
1939 C	1937	OD1	ASN	Α	367	-41.	.276	33.21	9 7	8.172	1.00	51.80
1940	1938	ND2	ASN	Α	367	-39.	.271			7.525	1.00	46.36
1941 N	1939	C	ASN	Α	367	-37.	.086	33.52	4 7	8.875	1.00	39.35
1942 CA	1940	0	ASN	Α	367			34.70			1.00	38.80
1943 CB		N	PRO	Α	368							39.49
1944 CG												
1945 CD		CB										
1946 C												
1948 N SER A 369 -37.064 33.502 75.664 1.00 42.38 1949 CA SER A 369 -37.639 34.437 74.597 1.00 43.38 1950 CB SER A 369 -39.639 32.601 73.740 1.00 42.38 1951 CS SER A 369 -39.033 33.951 74.203 1.00 44.88 1952 C SER A 369 -37.639 34.684 74.995 1.00 44.04 1953 CS SER A 369 -37.742 35.894 74.995 1.00 44.04 1953 CS SER A 369 -37.692 36.186 76.295 1.00 44.04 1955 CS GEN A 370 -37.692 36.186 76.295 1.00 44.21 1955 CS GEN A 370 -37.692 37.399 78.053 1.00 45.55 1955 CS GEN A 370 -38.437 37.399 78.053 1.00 45.55 1958 CS GEN A 370 -38.437 37.399 78.053 1.00 45.55 1959 CS GEN A 370 -40.602 37.264 79.300 1.00 56.48 1959 CS GEN A 370 -40.602 38.056 80.230 1.00 55.95 1961 CS GEN A 370 -36.232 38.251 76.902 1.00 44.24 19.30 1.00 40.424 19.404												
1948 N SER A 369 -37.064 33.592 75.664 1.00 42.38 1950 CB SER A 369 -37.083 34.437 74.597 1.00 43.99 1951 OG SER A 369 -39.033 33.951 74.203 1.00 44.98 1952 C SER A 369 -37.742 35.894 74.995 1.00 44.98 1953 O SER A 369 -37.742 35.894 74.995 1.00 44.29 1955 O SER A 369 -37.742 35.894 74.995 1.00 44.29 1955 CA GLN A 370 -37.692 36.186 76.295 1.00 44.21 1955 CA GLN A 370 -37.719 37.591 76.221 1.00 45.13 1955 CB GLN A 370 -38.437 37.397 78.053 1.00 45.51 1955 CB GLN A 370 -39.833 37.121 77.994 1.00 50.14 1958 CD GLN A 370 -40.602 37.244 79.300 50.44 1959 OE1 GLN A 370 -40.602 37.244 79.300 50.44 1950 OE GLN A 370 -40.602 37.246 79.300 1.00 55.95 1962 O GLN A 370 -36.210 30.956 80.230 1.00 55.95 1962 O GLN A 370 -36.210 30.956 80.230 1.00 55.95 1963 N AG A 371 -35.285 37.430 76.631 1.00 44.24 1965 CB ARG A 371 -35.285 37.430 76.631 1.00 43.01 1966 CG ARG A 371 -32.914 36.266 78.279 1.00 36.93 1967 CD ARG A 371 -32.118 35.265 78.279 1.00 36.93 1968 NE ARG A 371 -32.191 36.267 76.882 1.00 42.30 1970 NH1 ARG A 371 -32.513 32.243 77.663 1.00 43.01 1971 NH2 ARG A 371 -32.513 32.134 79.452 1.00 33.06 1972 C ARG A 371 -32.513 32.134 79.452 1.00 33.06 1973 O ARG A 371 -32.513 32.134 79.452 1.00 33.06 1973 O ARG A 371 -32.561 38.306 74.374 1.00 43.01 1971 NH2 ARG A 371 -32.561 38.306 74.374 1.00 43.01 1971 NH2 ARG A 371 -33.915 37.407 75.406 1.00 43.01 1973 O ARG A 371 -32.561 38.306 74.374 1.00 43.01 1974 N PO ARG A 372 -32.272 38.831 74.717 1.00 43.01 1975 CA PRO A 372 -32.678 40.611 74.274 1.00 43.01 1977 CR PRO A 372 -32.371 40.456 76.678 1.00 43.01 1978 CD PRO A 372 -32.371 40.456 76.678												
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1951												
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1954 N GLN A 370 -37.692 36.186 76.295 1.00 44.21 1955 CA GLN A 370 -37.719 37.519 76.721 1.00 45.55 1957 CG GLN A 370 -38.437 37.239 78.053 1.00 45.55 1958 CD GLN A 370 -40.602 37.264 79.300 1.00 56.14 1959 OEI GLN A 370 -40.602 37.264 79.301 1.00 56.38 1960 NEZ GLN A 370 -40.602 38.056 60.230 1.00 55.95 1961 C GLN A 370 -36.332 38.231 76.606 1.00 44.45 1962 O GLN A 371 -32.913 38.231 76.631 1.00 43.95 1965 CB ARG A 371 -												
1955 CA GLN A 370 -37,719 37,591 76,211 1.00 45,13 1956 CB GLN A 370 -38,437 37,739 78,053 1.00 45,513 1957 CG GLN A 370 -38,839 37,121 77,994 1.00 50,14 1958 CD GLN A 370 -40,602 37,264 79,300 1.00 56,48 1960 NE2 GLN A 370 -40,602 38,056 80,230 1.00 55,95 1961 C GLN A 370 -36,212 39,423 77,663 1.00 44,24 1963 N ARG A 371 -35,285 37,430 76,631 1.00 43,24 1964 CA ARG A 371 -32,118 37,962 76,693 1.00 43,01 1965 CB ARG A 371 -32,118 35,232 78,247 70,03 3,06 1966 CG ARG A 371 -32,118 35,232 78,247 1.00 33,06												
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1978 CD PRO A 372 -32.371 40.456 76.678 1.00 43.28 1979 C PRO A 372 -31.829 39.874 73.226 1.00 43.31	1976	CB	PRO	Α	372	-31.	.890	41.83	7 7	4.717	1.00	43.00
1979 C PRO A 372 -31.829 39.874 73.226 1.00 43.31	1977	CG	PRO	Α	372	-31.	.590	41.64	8 7	6.178	1.00	42.62
	1978	CD	PRO					40.45	6 7	6.678	1.00	43.28
1980 O PRO A 372 -31.191 38.862 73.545 1.00 43.24		C						39.87			1.00	43.31
	1980	0	PRO	Α	372	-31.	.191	38.86	2 7	3.545	1.00	43.24

FIGURE 3AM

A	В	С	D	Ε	F	G	H	1	J
1981	N	MET	Α	373	-31.820	40.378	71.995	1.00	43.19
1982	CA	MET		373	-30.928	39.857	70.976	1.00	43.50
1983	CB	MET			-31.448	40.174	69.585	1.00	44.61
1984	CG			373	-32.688	39.421	69.205	1.00	50.78
1985	SD			373	-33.173	39.941	67.576	1.00	64.15
1986	CE			373	-32.985	41.823	67.726	1.00	59.77
1987	C	MET	A	373	-29.564	40.516	71.172	1.00	42.00
1988	0	MET			-29.364	41.539	71.841	1.00	39.32
1989	N	LEU			-28.526	39.926	70.597		41.82
					-27.188		70.727	1.00	
1990	CA	LEU				40.488			43.13
1991	CB	LEU			-26.194	39.605	70.025	1.00	43.22
1992	CG	LEU			-25.814	38.411	70.923	1.00	45.40
1993	CD1	LEU			-24.780	37.453	70.278	1.00	44.95
1994	CD2	LEU			-25.284	38.861	72.288		41.96
1995	С	LEU			-27.192	41.923	70.171	1.00	43.85
1996	0	LEU			-26.478	42.788	70.667	1.00	43.31
1997	N	ALA		375	-27.951	42.152	69.118	1.00	43.58
1998	CA	ALA			-27.979	43.472	68.494	1.00	44.11
1999	CB	ALA			-29.028	43.491	67.388	1.00	43.88
2000	C	ALA			-28.336	44.516	69.517	1.00	43.69
2001	0	ALA			-27.783	45.616	69.548	1.00	45.16
2002	N	GLU			-29.265	44.123	70.370	1.00	43.44
2003	CA	GLU	Α	376	-29.855	44.996	71.354	1.00	43.12
2004	CB	GLU	Α	376	-31.147	44.357	71.836	1.00	43.67
2005	CG	GLU	Α	376	-32.103	44.068	70.705	1.00	49.90
2006	CD	GLU	Α	376	-33.520	43.811	71.206	1.00	57.55
2007	OE1	GLU	Α	376	-33.691	42.679	71.699	1.00	56.12
2008	OE2	GLU	Α	376	-34.454	44.705	71.124	1.00	60.58
2009	С	GLU	Α	376	-28.969	45.306	72.529	1.00	41.38
2010	0	GLU	Α	376	-29.116	46.343	73.152	1.00	42.50
2011	N	VAL	Α	377	-28.059	44.394	72.850	1.00	39.33
2012	CA	VAL	Α	377	-27.116	44.602	73.948	1.00	37.51
2013	CB	VAL	Α	377	-26.405	43.276	74.328	1.00	36.63
2014	CG1	VAL	Α	377	-25.281	43.536	75.284	1.00	35.55
2015	CG2	VAL	Α	377	-27.416	42.254	74.883	1.00	37.26
2016	С	VAL	Α	377	-26.043	45.547	73.449	1.00	37.40
2017	0	VAL	Α	377	-25.604	46.436	74.147	1.00	37.91
2018	N	LEU	Α	378	-25.621	45.323	72.219	1.00	37.51
2019	CA	LEU	Α	378	-24.580	46.115	71.589	1.00	39.81
2020	CB	LEU	Α	378	-24.266	45.532	70.217	1.00	40.42
2021	CG	LEU	Α	378	-23.393	44.286	70.335	1.00	41.70
2022	CD1	LEU	Α	378	-23.067	43.658	68.983	1.00	46.77
2023	CD2	LEU			-22.130	44.678	71.057	1.00	37.23
2024	C	LEU			-24.946	47.580	71.442		41.32
2025	o	LEU			-24.075	48.445	71.358	1.00	42.45
2026	N	GLU			-26.244	47.845	71.421	1.00	41.71
2027	CA	GLU		379	-26.719	49.178	71.213	1.00	42.63
2028	CB	GLU		379	-27.670	49.206	70.018	1.00	44.54
2029	CG	GLU			-26.995	48.791	68.724	1.00	47.20
2030	CD	GLU			-27.923	48.707	67.527	1.00	56.88
2031	OE1				-29.177	48.664	67.706	1.00	59.40
2001	CLI	020	-1	515	23.111	10.004	000	1.00	55.40

FIGURE 3AN

A	В	С	D	E		F		G	Н		1	J
2032	OE2	GLU	Α	379		-27.372	4	8.665	66.3	889	1.00	61.82
2033	C	GLU	Α	379		27.401	4	9.692	72.4	160	1.00	43.14
2034	0	GLU				-28.071		0.749	72.4		1.00	43.40
2035	N	HIS				-27.244		8.966	73.5		1.00	41.24
2036	CA			380		-27.851		9.440	74.7		1.00	40.10
2037	CB	HIS				-27.681		8.393	75.9		1.00	39.60
2038	CG	HIS				28.332		8.789	77.1		1.00	38.52
2039	ND1					-29.551		8.279	77.5		1.00	40.40
2040	CE1			380		29.890		8.824	78.7		1.00	37.68
2041	NE2	HIS				-28.923		9.643	79.1		1.00	39.48
2041	CD2					-20.923		9.644	78.1		1.00	34.37
2042	C C	HIS				27.942		0.747	75.1		1.00	
												39.36
2044	0	HIS				-25.985		0.841	75.0		1.00	39.34
2045	N	PRO				-27.882		1.732	75.7		1.00	40.21
2046	CA			381		-27.277		3.041	75.9		1.00	40.19
2047	CB	PRO				28.439		3.885	76.5		1.00	40.84
2048	CG			381		-29.677		3.167	76.0		1.00	42.96
2049	CD			381		-29.307		1.702	76.1		1.00	40.74
2050	С			381		-26.165		2.971	77.0		1.00	39.71
2051	0			381		-25.239		3.739	76.8		1.00	38.49
2052	N	TRP				-26.267		2.094	78.0		1.00	37.20
2053	CA	TRP				-25.213		1.967	79.0		1.00	36.17
2054	CB	TRP				-25.638		1.046	80.1		1.00	34.80
2055	CG			382		-24.604		0.947	81.2		1.00	35.01
2056	CD1	TRP				-24.349		1.852	82.1		1.00	36.17
2057	NE1	TRP	Α	382	-	-23.326	5	1.402	82.9	75	1.00	39.89
2058	CE2	TRP	Α	382	-	-22.895	5	0.191	82.5	05	1.00	36.83
2059	CD2	TRP	Α	382	-	23.684	4	9.879	81.3	91	1.00	34.51
2060	CE3	TRP	Α	382	-	23.437	4	8.680	80.7	16	1.00	37.27
2061	CZ3	TRP	Α	382	-	-22.450	4	7.843	81.1	.85	1.00	35.85
2062	CH2	TRP	Α	382	-	-21.675	4	8.196	82.2	83	1.00	34.82
2063	CZ2	TRP	Α	382	-	21.887	4	9.357	82.9	66	1.00	32.53
2064	C	TRP	Α	382	-	23.940	5	1.436	78.3	346	1.00	36.25
2065	0	TRP	Α	382	-	22.833	5	1.887	78.€	557	1.00	36.89
2066	N	ILE	Α	383	-	-24.090	5	0.456	77.4	172	1.00	36.03
2067	CA	ILE	Α	383	-	-22.943	4	9.924	76.7	34	1.00	36.79
2068	CB	ILE	Α	383	-	-23.373	4	8.683	75.8	392	1.00	36.16
2069	CG1	ILE	Α	383	-	23.751	4	7.476	76.8	302	1.00	34.61
2070	CD1	ILE	Α	383	-	-22.522	4	6.916	77.5	31	1.00	34.04
2071	CG2	ILE	Α	383		-22.221	4	8.209	75.0		1.00	35.05
2072	C			383		-22.377		1.014	75.8		1.00	39.31
2073	o			383		-21,172		1.250	75.7		1.00	40.13
2074	N	THR				-23.268		1.707	75.1		1.00	41.29
2075	CA	THR				-22.849		2.781	74.2		1.00	44.28
2076	CB			384		-24.120		3.418	73.6		1.00	44.01
2077	OG1	THR				-24.539		2.622	72.5		1.00	48.12
2078	CG2	THR				-23.822		4.750	73.0		1.00	49.09
2079	C			384		-22.006		3.846	74.8		1.00	43.49
2080	Ö	THR				-20.980		4.271	74.3		1.00	46.02
2081	N	ALA				-22.449		4.281	76.0		1.00	42.28
2082	CA	ALA				-21.779		5.332	76.7			42.24
2002	Ori	******	-1	555		21.115		0.002		00	1.00	24

FIGURE 3AO

A	В	С	D	E	F	G	H	1	J
2083	CB	ALA	Α	385	-22.705	55.884	77.823	1.00	41.95
2084	C	ALA			-20.509	54.897	77.424	1.00	42.41
2085	0	ALA			-19.606	55.728	77.660		43.21
2086	N	ASN			-20.404	53.612	77.749		40.11
2087	CA	ASN			-19.254	53.178	78.478		38.95
2088	CB	ASN			-19.696	52.453	79.740	1.00	39.05
2089	CG	ASN			-20.371	53.392	80.739	1.00	39.22
2090	OD1	ASN			-19.698	54.080	81.495	1.00	40.98
2091	ND2	ASN			-21.695	53.396	80.754		40.56
2091	C	ASN			-18.195	52.366	77.760	1.00	38.55
2092	0	ASN			-17.077	52.329	78.212	1.00	37.05
2093				387	-18.545	51.701	76.682	1.00	39.28
2094	N	SER			-17.604	50.833	75.997	1.00	41.73
	CA								
2096	CB	SER			-18.322	49.922	75.010		40.55
2097	OG			387	-17.359	49.075	74.356		42.67
2098	C			387	-16.573	51.578	75.172	1.00	43.18
2099	0			387	-16.930	52.538	74.482	1.00	43.25
2100	N			388	-15.344	51.059	75.181	1.00	44.22
2101	CA	SER			-14.244	51.555	74.351		46.24
2102	CB			388	-12.908	51.070	74.888		46.39
2103	OG			388	-12.725	51.591	76.195	1.00	49.91
2104	C			388	-14.358	51.150	72.894		46.36
2105	0			388	-15.115	50.231	72.549	1.00	48.50
2106		ADP			-9.414	25.400	78.378	1.00	
2107	PA	ADP			-9.486	25.363	79.862	1.00	30.26
2108		ADP			-10.590	26.255	80.350	1.00	
2109		ADP			-9.587	23.880	80.555	1.00	30.98
2110	PB	ADP			-10.917	23.134	80.991	1.00	31.28
2111		ADP			-11.692	24.139	81.826		28.29
2112		ADP			-10.390	21.986	81.811		35.80
2113		ADP			-11.688	22.740	79.755	1.00	28.57
2114	05*	ADP			-8.144	25.872	80.503	1.00	30.75
2115	C5*	ADP			-8.004	25.866	81.924	1.00	30.70
2116	C4*	ADP			-7.217	27.124	82.368		29.95
2117	04*	ADP			-5.951	27.178	81.679	1.00	28.79
2118	C1*	ADP	X2	2001	-5.642	28.545	81.342	1.00	29.10
2119	C2*	ADP			-6.747	29.415	81.899	1.00	26.58
2120	02*	ADP			-6.392	29.725	83.238	1.00	34.16
2121	C3*	ADP	X2	2001	-7.895	28.436	81.993		29.24
2122	03*	ADP	X2	2001	-8.952	28.763	82.864		32.70
2123	И9	ADP			-5.577	28.628	79.892	1.00	
2124	C8	ADP			-6.337	27.843	79.041	1.00	30.16
2125	N7	ADP	X2	2001	-6.028	28.206	77.750	1.00	29.74
2126	C5	ADP	X2	2001	-5.143	29.196	77.814	1.00	26.13
2127	C6	ADP	X2	2001	-4.519	29.877	76.813		29.08
2128	N6	ADP	X2	2001	-4.713	29.555	75.506	1.00	25.43
2129	C4	ADP	X2	2001	-4.835	29.464	79.141	1.00	28.26
2130	N3	ADP	X2	2001	-3.975	30.435	79.478	1.00	30.28
2131	C2	ADP	X2	2001	-3.350	31.144	78.490	1.00	31.73
2132	N1	ADP	X2	2001	-3.633	30.829	77.180	1.00	29.64
2133	0	HOH			-9.988	28.798	79.067		31.10

FIGURE 3AP

A	В	C	D	Е	F	G	F	I	1	J
2134	0	нон	х30	003	-14.393	22.868	80.	872	1.00	27.85
2135	0	HOH	X30	004	-13.728	20.345	80.	020	1.00	45.36
2136	0	HOH	X30	005	-26.951	31.694	86.	552	1.00	30.10
2137	Ó	HOH			-22.935	30.435		351	1.00	36.29
2138	o	НОН			-30.168	16.939		846		45.13
2139	o	нон			-18.066	25.328		601	1.00	31.20
2140	o	нон			-11.548	26.843		941	1.00	36.99
2141	0	НОН			-8.649	27.311		774	1.00	31.45
2142	0	нон			-37.854	36.557		013		38.02
2143	o	HOH			-27.723	38.845		275		37.13
2144	o	HOH			-16.636	24.694		361	1.00	32.
2145	o	HOH			-8.241	35.027		248	1.00	33.00
2146	o	HOH			-0.912	17.916		933	1.00	36.14
2147	ő	HOH			-15.066	34.944		120		42.99
2148	ő	нон			-22.824	25.783		176		46.76
2149	ő	нон			-11.944	23.669		418	1.00	39.47
2150	o	нон			-12.703	21.499		561		40.61
2151	o	нон			-37.367	42.995		960	1.00	59.45
2152	o	нон			-5.576	15.379		195		66.48
2153	o	HOH			-8.353	43.652		479		
2154	o	HOH			-23.236	19.714		938		47.17
2155	o	HOH			-10.809	32.568		377	1.00	35.26
2156	0	HOH			-15.673	31.938		442		44.34
2157	o	HOH			-0.223	35.059		257		55.88
2158	ő	нон			-20.254	50.297		242		49.49
2159	ő	нон			-4.408	26.185		520	1.00	57.94
2160	o	нон			-6.464	20.470		244		42.32
2161	o	НОН			-26.908	54.727		094	1.00	46.09
2162	0	нон			-3.500	31.862		803		43.64
2163	ō	HOH			-28.118	35.557		369	1.00	
2164	ō	HOH			-26.182	36.321		264	1.00	49.67
2165	ō	HOH			14.155	34.581		299		48.35
2166	ō	HOH			-34.861	43.555		702	1.00	53.19
2167	Ó	HOH			-39.173	35.975		307		45.97
2168	o	НОН			-14.153	39.758		741	1.00	38.14
2169	0	НОН	X30	044	-17.759	51.104	95.	196	1.00	63.77
2170	0	HOH			-17.674	46.814		492	1.00	55.41
2171	0	HOH			-21.016	27.883		182	1.00	40.34
2172	0	HOH			-32.376	28.743		835	1.00	35.07
2173	0	HOH	х30	048	-26.582	54.610	84.	614	1.00	51.10
2174	0	HOH	X30	049	-28.989	37.779	69.	028	1.00	45.59
2175	0	HOH	X30	050	1.044	35.132	80.	541		40.83
2176	0	HOH	X30	051	-18.143	48.279	89.	631	1.00	35.13
2177	0	HOH	X30	052	-22.772	50.169	87.	633	1.00	35.90
2178	0	HOH	X30	054	-28.242	40.105	67.	233	1.00	39.46
2179	0	HOH	X30	055	-5.648	27.887	86.	644	1.00	45.28
2180	0	HOH	X30	056	-22.278	29.579	81.	107	1.00	46.99
2181	0	HOH			-21.804	27.943		859	1.00	31.17
2182	0	HOH			-19.327	55.542	84.	158		69.06
2183	0	HOH	Х30	059	-16.658	53.812	86.	138	1.00	76.39
2184	0	HOH	X30	060	-11.616	48.407	86.	048	1.00	44.96

FIGURE 3AQ

A	В	С	D	E	F	G	H	I	J
2185	0	нон	va	061	-35.280	41.364	78.456	1.00	43.63
2186	0	HOH			-35.848	29.209	81.326	1.00	50.09
2187	0	HOH			-20.386	19.911	74.001	1.00	46.93
2188	0	HOH			-5.444	37.823	84.054	1.00	35.84
2189	0	НОН			-2.738	38.173	71.721	1.00	47.11
2190	0	НОН			-3.973	35.760	72.248	1.00	33.90
2191	0	HOH			-29.746	39.136	96.635	1.00	62.80
2192	Ö	HOH			-14.064	25.472	82.227	1.00	31.69
2193	Ö	HOH			-4.484	33.261	84.056	1.00	47.20
2194	ō	нон	X2	090	-9.895	27.055	74.329	1.00	27.24
2195	ō	HOH			-0.170	31.678	70.061	1.00	29.25
2196	0	HOH	Х2	092	-1.106	31.853	83.735	1.00	53.32
2197	o	нон	Х2	093	-25.264	41.053	66.798	1.00	59.10
2198	0	HOH	Х2	094	-25.466	43.888	65.479	1.00	69.73
2199	0	HOH	Х2	095	-32.272	31.292	69.214	1.00	67.50
2200	0	HOH	Х2	096	-24.385	33.367	89.916	1.00	31.89
2201	0	HOH	Х2	097	-14.677	21.587	82.263	1.00	41.33
2202	0	HOH	X2	098	-15.335	22.257	78.530	1.00	36.43
2203	0	HOH	X2	099	-11.146	29.804	67.165	1.00	47.94
2204	0	HOH	Х2	100	-9.610	28.214	65.560	1.00	46.43
2205	MG	MG	Х2	086	-13.528	22.597	79.198	1.00	12.09
2206	MG	MG	Х2	880	-12.337	25.921	81.074	1.00	12.20
2207	P	PO4		002	-24.838	17.852	76.312	1.00	54.63
2208	01	PO4	Х2	002	-24.694	18.499	74.963	1.00	59.50
2209	02	PO4		002	-26.204	17.207	76.361	1.00	64.72
2210	03	PO4		002	-23.779	16.793	76.532	1.00	57.00
2211	04	PO4	X2	002	-24.798	18.859	77.420	1.00	60.01